Ukrainian Conference with International Participation

«CHEMISTRY, PHYSICS AND TECHNOLOGY OF SURFACE»

and

Workshop

«METAL-BASED BIOCOMPATIBLE NANOPARTICLES: SYNTHESIS AND APPLICATIONS»

15 - 17 May 2019
Kyiv
Ukraine

National Academy of Sciences of Ukraine
Chemistry Division
Chuiko Institute of Surface Chemistry
Scientific Council
"Chemistry and Technology of Surface Modification"

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METAL-BASED BIOCOMPATIBLE NANOPARTICLES: SYNTHESIS AND APPLICATIONS

Book of abstracts

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Матеріали Всеукраїнської конференції з міжнародною участю «Хімія, фізика і технологія поверхні» і семінару «Синтез та застосування біосумісних наносистем на основі металів» – Київ, 2019. – 232 с.

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Збірник містить тези доповідей, які було представлено на конференції і семінарі. Тематика конференції: теорія хімічної будови та реакційна здатність поверхні твердих тіл; фізико-хімія поверхневих явищ; хімія, фізика та технологія наноматеріалів; медико-біологічні та біохімічні аспекти дослідження високодисперсних матеріалів. Тези доповідей подано в авторській редакції.

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Scientific Council "Chemistry and Technology of Surface Modification"

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Conference Program

May 15, Wednesday

9:00 – 9:45 Registration of Participants

10:00 – 10:20 Opening of the Conference at the Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine
Academician of NAS of Ukraine, Professor M. Kartel

Oral Session 1
Chair: Professor M. Kartel

10:20 – 10:50 M. Larsson. **The 1932 Nobel Prize in Chemistry: Irving Langmuir** (*Stockholm University, AlbaNova University Center, Department of Physics, Sweden*).

10:50 – 11:20 V.M. Gun'ko. **Theoretical analysis of adsorption of various compounds onto hydrophilic and hydrophobic silicas** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

11:20 – 11:30 Group Photo

11:30 – 11:50 Coffee Break

Oral Session 2
Chair: Professor V. Tertykh

11:50 – 12:10 V.P. Grankin, D.V. Grankin. **Accommodation of the reaction energy by the electron channel on the surface of planar heterostructures** (*Pryazovskyi State Technical University, Mariupol, Ukraine*).

12:10 – 12:30 G.A. Seisenbaeva[1], V.G. Pol[2]. **Mesoporous metal oxide anodes for Li-ion batteries** (*[1]Department of Molecular Sciences, Swedish University of Agricultural Sciences, Uppsala, Sweden, [2]Davidson School of Chemical Engineering, Purdue University, West Lafayette, USA*).

12:30 – 12:45 A. Ievtushenko[1], M. Dusheiko[2], S. Mamykin[3], V. Koval[2], O. Olifan[1], O. Kolomys[3], S. Korichev[1], V. Strelchuk[3], V. Tkach[4]. **The effect of substrate temperature and air annealing on the structure, optical and electrical properties of MoO_x thin films deposited by reactive ion-beam sputtering** (*[1]Frantsevich Institute for Problems of Material Science, NAS of Ukraine, Kyiv, [2]National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", [3]V.E. Lashkarev Institute of Semiconductor Physics, NAS of Ukraine, Kyiv, [4]V. Bakul Institute for Superhard Materials, NAS of Ukraine, Kyiv*).

12:45 – 12:55 **P.V. Torchyniuk**, O.I. V'yunov, A.G. Belous. **Synthesis of nanosized organic-inorganic perovskite films $CH_3NH_3PbI_3$: effect of initial reagents ratio on formation and microstructure** (*Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Kyiv*).

12:55 – 13:05 **O.P. Fedorchuk**, S.O. Solopan, Yu.D. Stupin, B.S. Khomenko. **Influence of synthesis conditions on the physical and chemical properties of the yttrium iron garnet** (*Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Kyiv*).

13:05 – 14:00 Break

Oral Session 3

Chair: ***Professor V. Gun'ko***

14:00 – 14:15 **I.V. Romanova**[1], S.A. Kirillov[2]. **Modified citric method for obtaining of functional oxide materials** (*[1]Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv, [2]Joint Department of Electrochemical Energy Systems, NAS of Ukraine, Kyiv*).

14:15 – 14:30 **K.V. Voitko**, E.M. Demianenko, V.S. Kuts, O.M. Bakalinska, M.T. Kartel. **Catalytic decomposition of organic/inorganic peroxides by carbon matrix: experimental and quantum-chemical investigation** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

14:30 – 14:45 **S.O. Zelinskyi**, Y.A. Maletin, N.G. Stryzhakova, O.V. Gozhenko. **Modification of nanoporous structure and surface of carbon materials to be used in energy storage technology** (*Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv*).

14:45 – 15:00 **V.V. Shvalagin**, A.V. Korzhak, S.Ya. Kuchmiy. **Composite nanostructures based on crystalline graphitic carbon nitride for efficient photocatalytic hydrogen production under visible light** (*L.V. Pisarzhevskii Institute of Physical Chemistry, NAS of Ukraine, Kyiv*).

15:00 – 15:15 **M. Bondarenko**, P. Silenko, Yu. Solonin, N. Gubareni, O. Khyzhun, N. Ostapovskaya. **Synthesis $O\text{-}g\text{-}C_3N_4/TiO_2$ rutile composite material for photocatalytic application** (*Frantsevich Institute for Problems of Materials Science, NAS of Ukraine, Kyiv*).

15:15 – 15:25 **O. Sanzhak**[1], D. Brazhnyk[1], V. Goncharov[2], V. Zazhigalov[1], F. Azimov[1]. **Synthesis of Ti-containing photocatalyst supported on stainless steel** (*[1]Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv, [2]State Establishment "Lugansk State Medical University", Rubizhne, Ukraine*).

15:25 – 15:35 **M. Samsonenko**[1], S. Khalameida[1], L. Kotynska[1], V. Permyakov[2], S. Shcherbakov[3]. **The study of photocatalytic properties of doped tin oxide prepared by sonochemical method** (*[1]Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv, [2]Institute of Geological Sciences, NAS of Ukraine, Kyiv, [3]M.G. Kholodny Institute of Botany, NAS of Ukraine, Kyiv*).

15:35 – 15:45 O.P. Pertko, Yu.G. Voloshyna, L.K. Patrylak. **The influence of external surface modification on the zeolite catalysts coking** (*V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry, NAS of Ukraine, Kyiv*).

15:45 – 15:55 N.V. Diyuk[1], O.V. Sachuk[2], V.O. Zazhigalov[2], V.L. Starchevskyy[3]. **H_2 – TPR characterization of $ZnMoO_4$ obtained by ultrasonic method** ([1]*Taras Shevchenko National University of Kyiv, Ukraine,* [2]*Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv,* [3]*National University «Lviv Polytechnic», Ukraine*).

15:55 – 16:05 M. Sęczkowska[1], M.V. Galaburda[2], V.M. Bogatyrov[2], A. Deryło-Marczewska[1], A.W. Marczewski[1]. **Active carbons from nutshells – preparation, properties and application** ([1]*Faculty of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland,* [2]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

16:05 – 16:15 O.A. Cherniuk[1], G.I. Dovbeshko[2], S.V. Zhuravskyi[1], S.M. Makhno[1], M.T. Kartel[1], Yu.I. Sementsov[1]. **Study of glass-reinforced plastic filled by surface modified multiwall carbon nanotubes** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*Department of Physics of Biological Systems, Institute of Physics, NAS of Ukraine, Kyiv*).

16:15 – 16:35 Coffee Break

16:35 – 17:30 ***Poster Session I (1-82)***

May 16, Thursday

Oral Session 4

Chair: Professor V. Rozenbaum

10:00 – 10:20 S.I. Pokutnyi. **Stationary and quasistationary electron states in quasiatomic nanosystems** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

10:20 – 10:35 T.Ye. Korochkova[1], V.M. Rozenbaum[1], U.A. Vysotskaya[2], E.V. Shakel[3]. **Temperature dependence of a particle flux in a Brownian ratchet with slightly fluctuating potential energy** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*Belarusian State University, Minsk,* [3]*National Institute for Higher Education, Minsk, Belarus*).

10:35 – 10:55 A.N. Herega[1], Yu.V. Kryvchenko[2]. **The new reinforcement technology of concrete as the new percolation problem** ([1]*Research and Production Center, Odessa,* [2]*Odessa National Academy of Food Technologies, Ukraine*).

10:55 – 11:10 I.V. Melnyk[1,2], V.V. Tomina[2], N.V. Stolyarchuk[2], I.M. Furtat[3], M. Vaclavikova[1]. **Controllable design of aminosilica microparticles for multi-uses** ([1]*Institute of Geotechnics, Slovak Academy of Sciences, Kosice,* [2]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [3]*National University of Kyiv-Mohyla Academy, Ukraine*).

11:10 – 11:25 **H. Vasylyeva**[1], I. Myroniuk[2], I. Mykytyn[2]. **Adsorption of Co^{2+} cations and radioactive ^{60}Co by mesoporous TiO_2** ([1]*Uzhgorod National University, Ukraine,* [2]*Vasyl Stefanyk Precarpathian National University, Ivano-Frankivsk, Ukraine*).

11:25 – 11:45 Coffee Break

Oral Session 5
Chair: Dr. (Chem.) O. Linnik

11:45 – 12:00 **Iu. Mukha**[1], N. Vityuk[1], A. Eremenko[1], V. Lysenko[2], M. Lokshyn[2]. **Formation of gold nanoparticles in $HAuCl_4$ / Na citrate system depending on concentration of components, temperature and pH** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*V.E. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, Kyiv*).

12:00 – 12:15 **I.V. Pylypchuk**[1,2], V.G. Kessler[1], G.A. Seisenbaeva[1]. **Development of multifunctional enzyme-bearing magnetic nanocomposites** ([1]*Department of Molecular Sciences, Swedish University of Agricultural Sciences, Uppsala,* [2]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

12:15 – 12:30 **N.M. Rusinchuk**[1], V.Z. Lozovski[1], V.S. Lysenko[2]. **Antiviral properties of nanoparticles from the physical point of view** ([1]*Institute of High Technologies, Taras Shevchenko National University of Kyiv, Ukraine,* [2]*V.E. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, Kyiv*).

12:30 – 12:40 **M. Chaika**[1], O. Zaychenko[1], Yu. Pankivska[2], S. Zagorodnya[2], I. Mukha[3], N. Vityuk[3]. **Use of gold nanoparticles of different sizes, as potential antiviral agents** ([1]*ESC "Institute of Biology and Medicine", Taras Shevchenko National University of Kyiv, Ukraine,* [2]*Zabolotny Institute of Microbiology and Virology, NAS of Ukraine, Kyiv,* [3]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

12:40 – 12:50 **A. Khodko**[1], Iu. Mukha[2], N. Vityuk[2], V. Khomenko[1], A. Mamuta[1], N. Kachalova[1,3], A. Eremenko[2]. **Photoinduced synthesis of Ag(Au)/tryptophan nanoparticles by UV-C LEDs sources** ([1]*Institute of Physics, NAS of Ukraine, Kyiv,* [2]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [3]*L.M. Litvinenko Institute of Physical-Organic and Coal Chemistry, NAS of Ukraine, Kyiv*).

12:50 – 13:00 **I. Timashkov**, Yu. Shlapa, S. Solopan, A. Belous. **Microemulsion synthesis of CeO_2 nanoparticles and their properties** (*Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Kyiv*).

13:00 – 14:00 Break

Oral Session 6
Chair: ***Professor V. Turov***

14:00 – 14:20 F. Meng[1,2], M. Seredych[1], C. Chen[1,3], V. Gura[4], **S. Mikhalovsky**[5,6], S. Sandeman[6], G. Ingavle[6,7], T. Ozulumba[6], L. Miao[3], B. Anasori[1], Y. Gogotsi[1]. **MXene sorbents for removal of urea from dialysate – a step towards the wearable artificial kidney** ([1]*Drexel University, Philadelphia, USA,* [2]*Guangxi Medical University, Nanning, People's Republic of China,* [3]*Huazhong University of Science and Technology, Wuhan, People's Republic of China,* [4]*UCLA The David Geffen School of Medicine, Beverly Hills, USA,* [5]*University of Brighton, UK,* [6]*ANAMAD Ltd, Brighton, UK,* [7]*Symbiosis International University, Lavale, Pune, India*).

14:20 – 14:35 **R.M. Chornopyshchuk**[1], O.S. Kukolevska[1], V.I. Nagajchuk[1], I.I. Gerashchenko[2]. **Experimental study of composite material on polymeric basis which possesses antimicrobial activity** ([1]*Vinnytsia National Pirogov Memorial Medical University, Ukraine,* [2]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

14:35 – 14:50 **V.L. Demchenko**[1], S.V. Riabov[1], N.P. Rybalchenko[2], A.S. Kruk[3], O.V. Moskalenko[3]. **Structure, morphology and antimicrobial properties of silver-containing nanocomposites** ([1]*Institute of Macromolecular Chemistry, NAS of Ukraine, Kyiv,* [2]*Zabolotny Institute of Microbiology and Virology, NAS of Ukraine, Kyiv,* [3]*Nizhyn Mykola Gogol State University, Ukraine*).

14:50 – 15:05 **M. Studziński**[1], I. Malinowska[1], Y.M. Bolbukh[2], V.A. Tertykh[2]. **Investigation of drug desorption from carbon nanotubes and their chitosan composites to simulated body fluid** ([1]*Planar Chromatography Department, Chair of Physical Chemistry, Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland,* [2]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

15:05 – 15:15 A.L. Petranovska[1], M.V. Abramov[1], **N.M. Opanashchuk**[1], N.V. Kusyak[2], A.P. Kusyak[2], S.P. Turanska[1], S.V. Gorobets'[3], P.P. Gorbyk[1], N.Yu. Lukianova[4], V.F. Chekhun[4]. **Magnetically sensitive nanocomposites and magnetic fluids based on magnetite, gemcitabine and HER2 antibody** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*Ivan Franko Zhytomyr State University, Ukraine,* [3]*National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute",* [4]*R.E. Kavetsky Institute of Experimental Pathology, Oncology and Radiobiology, NAS of Ukraine, Kyiv*).

15:15 – 15:25 **V.V. Paientko**[1], A.K. Matkovsky[1], L.M. Babenko[2], O.I. Oranska[1], I.M. Chyrkov[3], V.M. Gun'ko[1]. **Composite fillers based on clay/nanosilica blends for cosmetic applications** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*Department of Phytohormonology, M.G. Kholodny Institute of Botany, NAS of Ukraine, Kyiv,* [3]*"ALEOL" LTD, Kyiv, Ukraine*).

15:25 – 15:45 Coffee Break

15:45 – 16:45 ***Poster Session II (83-163)***

17:00 – 17:15 Conference Closing

17:15 Post-Conference Reception

May 17, Friday

9:00 – 19:00 Outing Session (outside the city)

Poster Presentation

1. Theory of Chemical Structure and Reactivity of Solid Surface

1. **Y.S. Boiko**[1,3], O.A. Yesypenko[1], A.B. Drapailo[2], K.Yu. Bryleva[1], S.V. Sishkina[2], K.M. Byelikov[2], P.V. Vakuliuk[3], R.V. Rodik[1], O.A. Golub[3], V.I. Kalchenko[1]. **Modification of silica gel with tetraphosphorylated calix[4]arenes and examination of Eu(III) sorption** ([1]*Institute of Organic Chemistry, NAS of Ukraine, Kyiv,* [2]*State Scientific Institution "Institute for Single Crystals", NAS of Ukraine, Kharkiv,* [3]*National University of Kyiv-Mohyla Academy, Ukraine*).
2. W. Rettig[1], **M. Dekhtyar**[2]. **S_0-S_1 conical intersections of conjugated compounds** ([1]*Institut für Chemie, Humboldt-Universität zu Berlin, Germany,* [2]*Institute of Organic Chemistry, NAS of Ukraine, Kyiv*).
3. **A.B. Drapailo**[1], G.D. Yukhno[2], A.P. Krasnopyorova[2], N.V. Efimova[2], V.Yu. Korovin[3], O.V. Zontov[4], V.I. Kalchenko[1]. **Synthesis and properties of thiacalixarene based solid extractants for cerium(III) binding** ([1]*Institute of Organic Chemistry, NAS of Ukraine, Kyiv,* [2]*V.N. Karazin Kharkiv National University, Ukraine,* [3]*Institute of Geotechnical Mechanics named by N. Poljakov, NAS of Ukraine, Dnipro,* [4]*SE SMOLY, Kamyanske, Ukraine*).
4. V.V. Pototskaya[1], **O.I. Gichan**[2]. **New insight into the physical origin of phase angle in Warburg finite length diffusion impedance** ([1]*Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Kyiv,* [2]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
5. **D.S. Kamenskyh**, V.A. Yevdokymenko, T.V. Tkachenko, R.V. Korzh, V.I. Kashkovsky. **Lower olefines obtaining over membrane composite catalysts** (*V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry, NAS of Ukraine, Kyiv*).
6. **D.B. Nasiedkin**, A.G. Grebenyuk, Yu.V. Plyuto. **DFT study of hydrogen interaction with sulfur moieties in natural graphite** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
7. **O. Sevastyanova**[1], V. Turov[2], V. Gun'ko[2]. **Interfacial behavior of water bound to lignin particles** ([1]*Department of Fiber and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden,* [2]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
8. **M. Vorokhta**[1], I. Khalakhan[1], P. Hozák[2], J. Vlček[2], P. Fitl[2], M. Vrňata[2], M. Vondráček[3], J. Lančok[3], V. Matolín[1]. ***Operando* studies of the catalytic and gas sensing properties of nanostructured copper and tin oxide layers** ([1]*Department of Surface and Plasma Science, Charles University, Prague, Czech Republic,* [2]*Department of Physics and Measurements, Institute of Chemical Technology, Prague, Czech Republic,* [3]*Institute of Physics, Academy of Sciences of the Czech Republic, Prague*).

2. Physical Chemistry of Surface Phenomena

9. **A.B. Abdikamalova**, A.I. Sharipova. **Effects of synthesized polyelectrolytes on structure formation in soil dispersions** (*Faculty of Chemical Technology, Karakalpak State University, Nukus, Uzbekistan*).
10. **R.H. Amirov**, S.V. Sologub, I.V. Bordeniuk, T.V. Afanasieva. **Comparative investigation of scattering of conduction electrons on adsorbed submonolayers of hydrogen and deuterium** (*Institute of Physics, NAS of Ukraine, Kyiv*).

11. **D.Yu. Balakin**, T.V. Afanasieva, A.G. Fedorus, L.Yu. Lopandia, A.O. Stetcyuk, Yu.O. Mitryayeva. **Effect of oxygen adsorption on the thermal stability of beryllium nanolayers on the Mo (110) surface** (*Institute of Physics, NAS of Ukraine, Kyiv*).
12. **M. Blachnio**[1], A. Derylo-Marczewska[1], B. Charmas[1] M. Zienkiewicz-Strzałka[1], V. Bogatyrov[2], M. Galaburda[2]. **Active carbon from agricultural wastes for adsorption of organic pollutants** (*[1]Faculty of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
13. **M. Blachnio**[1], A. Derylo-Marczewska[1], B. Charmas[1], M. Zienkiewicz-Strzałka[1], V. Bogatyrov[2], M. Galaburda[2]. **Studies of thermal behavior of adsorbed organic pollutants on activated carbon** (*[1]Faculty of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
14. **A.I. Bondarieva**, Yu.M. Kholodko, V.Yu. Tobilko. **Removal of arsenic(V) from contaminated water with palygorskite supported hydrated Fe(III) oxides** (*National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"*).
15. **S. Burian**[1], O. Hrebnov[1], V. Sysoev[1], M. Isaiev[1,2]. **The contact angle of nanodroplets** (*[1]Faculty of Physics, Taras Shevchenko National University of Kyiv, Ukraine, [2]LEMTA, Université de Lorraine, CNRS (UMR 7563), Vandoeuvre-lès-Nancy, France*).
16. **O.A. Dudarko**[1], N.G. Kobylinska[2], V.A. Tertykh[1]. **Adsorption-structural properties of P-containing SBA-15 silicas** (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]Faculty of Chemistry, Taras Shevchenko National University of Kyiv, Ukraine*).
17. **O.A. Dudarko**[1], N.V. Stolyarchuk[1], V.V. Tomina[1], B.P. Tripathi[2]. **Creation of novel organic-inorganic hybrid materials as sorbents for wastewater treatment from heavy metal ions** (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]Indian Institute of Technology Delhi, New Delhi, India*).
18. **L.S. Dzubenko**[1], O.O. Sapyanenko[1], P.P. Gorbyk[1], S.V. Saitarly[2], V.P. Plavan[2], Yu.O. Budash[2]. **The highly-filled and polypropylene-based composites** (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]Kyiv National University of Technologies and Design, Ukraine*).
19. **N.V. Efimova**[1], A.P. Krasnopyorova[1], G.D. Yukhno[1], D.S. Sofronov[2], O.S. Kogol[1]. **Sorption of ^{110}Ag by MnO(OH) particles from aqueous solutions** (*[1]Faculty of Chemistry, V.N. Karazin Kharkiv National University, Ukraine, [2]State Scientific Institution «Institute for Single Crystals», NAS of Ukraine, Kharkiv, Ukraine*).
20. **V.V. Halysh**[1,2], Y. Zhang[3,4], O. Sevastyanova[3,4] . **Low-cost sorbents for the adsorption of pharmaceuticals** (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", [3]KTH Royal Institute of Technology, Department of Fiber and Polymer Technology, Stockholm, Sweden, [4]KTH Royal Institute of Technology, Wallenberg Wood Science Center, Stockholm, Sweden*).
21. V. Sydorchuk[1], **S. Khalameida**[1], O.I. Poddubnaya[1], M.M. Tsyba[1], O. Khyzhun[2], A.M. Puziy[1]. **Photocatalytic degradation of dyes using phosphorus-containing active carbons** (*[1]Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv, [2]Frantsevych Institute for Problems of Materials Science, NAS of Ukraine, Kyiv*).
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3. Chemistry, Physics and Technology of Nanomaterials

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102. **Yu. Pirskyy**[1], F. Manilevich[1], T. Panchyshyn[1], Ya. Kolosovskiy[2]. **Bifunctional iridium electrocatalysts for modifying surface of fuel cell proton-conducting membranes** ([1]*Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Kyiv,* [2]*Private Joint-Stock Company "ELMIZ", Kyiv, Ukraine*).
103. **E.N. Poddenezhny**, O.V. Davydova, N.E. Drobyshevskaya, A.A. Boiko. **Synthesis of nanostructure yttrium-aluminum garnet powders activated with cerium, europium, gadolinium and their luminescent characteristics** (*Sukhoi Gomel State Technical University, Belarus*).
104. **S.L. Prokopenko**, R.V. Mazurenko, G.M. Gunya, S.N. Makhno, P.P. Gorbyk. **Electrophysical properties of polychlorotrifluoroethylene nanocomposites based on calcium iron oxide modified copper sulfide** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
105. P.P. Gorbyk, S.M. Makhno, I.V. Dubrovin, O.M. Lisova, R.V. Mazurenko, **S.L. Prokopenko**, M.V. Abramov, S.P. Turanska, N.M. Opanashchuk. **Synthesis and properties of nanostructures absorbing ultrahigh-frequency electromagnetic and neutron radiation** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
106. L.N. Puzyrnaya, B.P. Yatsyk, **G.N. Pshinko**. **Composites based on layered double hydroxides – sorbents for the recovery uranium(VI)** (*Dumansky Institute of Colloid and Water Chemistry, NAS of Ukraine, Kyiv*).
107. **A.V. Redkina**, N.V. Kravchenko, N.D. Konovalova, V.V. Strelko. **Comparison of the influence of hydro-and alco-thermal treatment on the structure of zirconium silicate** (*Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv*).
108. **V.O. Sabierova**, Yu.V. Tamarkina, V.O. Kucherenko. **Coal transformation into nanoporous carbon under heat-shock alkali activation** (*L.M. Litvinenko Institute of Physical-Organic and Coal Chemistry, NAS of Ukraine, Kyiv*).
109. **M. Sęczkowska**, A. Deryło-Marczewska. **Active carbons with pharmaceutical use: structural and adsorption properties** (*Faculty of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland*).
110. **N.V. Sigareva**, E.P. Voronin, L.V. Nosach, B.M. Gorelov, O.V. Mischanchuk, D.L. Starokadomskiy. **Thermophysical properties of epoxy composites with modified nanosilica particles** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

111. **O.G. Sirenko**, S.M. Makhno, O.M. Lisova, G.M. Gunya, P.P. Gorbyk. **Electrophysical properties of composites based on epoxy resin and carbon nanotubes** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
112. **A.A. Shapoval**[1], Y.M. Panov[2], I.V. Shapoval[1], O.S. Ditkivska[2]. **Porous coatings and structures for the intensification of boiling processes on metallic heat-stressed surfaces** ([1]*Frantsevich Institute for Problems of Materials Science, NAS of Ukraine, Kyiv,* [2]*National Technical University of Ukraine «Igor Sikorsky Kyiv Polytechnic Institute»*).
113. **M.V. Shapovalova**, T.A. Khalyavka, S.V. Camyshan. **The influence of titanum dioxide modification with sulfur and carbon on its physico-chemical and photocatalytic properties** (*Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv*).
114. **H. Shymanskaya**[1], R. Papou[1], N. Sdobnyakov[2], D. Sokolov[2]. **Solution combustion synthesis of bimetallic and metal-ceramic nanomaterials** ([1]*Chemical Technology and Engineering Faculty, Belarusian State Technological University, Minsk,* [2]*Physico-Technical Faculty, Tver State University, Russia*).
115. **H.M. Starukh**. **ZnAl layered double hydroxides for absorption and photocatalytic removal of tetracycline antibiotics** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
116. **V.A. Stolbovoy**, I.V. Serdiuk, D.V. Vinnikov, A.V. Dolomanov. **Development of methods for applying titanium coatings on the elements of friction nodes of joint prostheses** (*National Science Center "Kharkov Institute of Physics and Technology", NAS of Ukraine*).
117. **N.V. Stolyarchuk**[1], V.V. Tomina[1], A. Beganskienė[2], A. Katelnikovas[2], M. Vaclavikova[3], A. Kareiva[2], I.V. Melnyk[1,3]. **Fabrication of improved rare-earth (Eu) complexes-embedded aminosilica microparticles** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*Vilnius University, Lithuania,* [3]*Institute of Geotechnics, Slovak Academy of Sciences, Kosice*).
118. **I. Sulym**[1], D. Sternik[2], Yu. Sementsov[1], S. Makhno[1], A. Derylo-Marczewska[2], B. Kalska-Szostko[3]. **Textural and structural characterization of carbon nanotubes/poly(dimethylsiloxane) composites** ([1]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv,* [2]*Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland,* [3]*Institute of Chemistry, Faculty of Biology and Chemistry, Univesity of Białystok, Poland*).
119. **O.A. Syvolozhskyi**[1], I.V. Ovsiienko[1], L.Yu. Matzui[1], A.G. Dyachenko[2], O.V. Ischenko[2], O.S. Yakovenko[1]. **Transport properties of nanographite modified with nickel and iron** ([1]*Faculty of Physics,* [2]*Faculty of Chemistry, Taras Shevchenko National University of Kyiv, Ukraine*).
120. E.M. Demianenko, **M.I. Terets**, Yu.I. Sementsov, A.G. Grebenyuk, M.T. Kartel. **Theoretical study on the effect of carbon nanotubes on the strength of covalent bonds of nylon in a nanocomposite** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
121. **O.I. Tkachuk**, M.I. Terebinska, V.V. Lobanov. **Diffusion and rotation of clean >Ge=Ge< and mixed >Ge=Si< addimers on bucled face Si(001)(4×2)** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
122. **G.P. Tsintskaladze**, L.G. Eprikashvili, T.V. Sharashenidze, V.M. Gabunia, N.V. Pirtskhalava, M.A. Dzagania. **Zeolite anion-containing nanoporous materials, prospects their production and use** (*Petre Melikishvili Institute of Physical and Organic Chemistry, Ivane Javakhishvili Tbilisi State University, Georgia*).

123. **N. Uludag. An efficient synthesis of nitriles and nitrile-containing pharmaceuticals** (*Faculty of Arts and Sciences, Department of Chemistry, Tekirdağ Namık Kemal University, Turkey*).
124. **V.V. Voloshchuk**, G.V. Lisachuk, R.V. Krivobok, A.V. Zakharov, L.S. Limarenko, P.P. Vabishchevich. **Technology for the production of complex products based on celsian ceramics** (*National Technical University "Kharkiv Polytechnic Institute", Ukraine*).
125. **V.S. Vorobets**, G.Ya. Kolbasov, S.Ya. Oblovatna, O.O. Salamakha, S.V. Karpenko, I.A. Rusetskyi. **Synthesis, photo- and electrocatalytic properties of nanostructured TiO$_2$-Ce films** (*Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Kyiv*).
126. **O.S. Yakovenko**, L.Yu. Matzui, L.L. Vovchenko, I.V. Ivakhov, O.V. Turkov, Y.S. Perets, A.V. Zhuravkov, T.A. Len. **Dielectric properties of hybrid carbon-based composite materials and composites with titanium dioxide** (*Faculty of Physics, Taras Shevchenko National University of Kyiv, Ukraine*).
127. **V.F. Zinchenko**[1], G.V. Volchak[1], O.G. Ieriomin[1], I.V. Stoyanova[1], N.O. Chivireva[1], S.V. Kuleshov[2], P.G. Doga[1]. **Spectral properties of ultra-dispersed systems of LaF$_3$ and EuF$_3$ in the stiffened melt NaCl-KCl** ([1]*A.V. Bogatsky Physico-Chemical Institute, NAS of Ukraine, Odesa,* [2]*Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Kyiv*).
128. **N.V. Zhdanyuk**, O.V. Shcherban. **Synthesis and characteristics of iron-containing nanocomposites based on palygorskite** (*National Technical University of Ukraine «Igor Sikorsky Kyiv Polytechnic Institute»*).
129. **M.O. Zoziuk**. **Analysis of the properties of some photorefractive organic materials for dynamic holography** (*National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"*).

4. Medical, Biological and Biochemical Aspects of Research of Highly Disperse Materials

130. **A.N. Bagatskaya**, R.V. Mazurenko, N.V. Abramov, S.N. Makhno, P.P. Gorbik. **Influence of endogenous metabolism of yeast *Saccharomyces cerevisiae* in magnetite-based magnetic fluid** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
131. **A.A. Boiko**[1], E.N. Poddenezhny[1], O.V. Davydova[1], N.E. Drobyshevskaya[1], M.V. Borysenko[2]. **Biodegradable composite materials on base of cellulose acetate** ([1]*Sukhoi Gomel State Technical University, Belarus,* [2]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
132. **O.G. Bordunova**[1], O.O. Chekh[1], E.G. Astrakhantseva[1], O.S. Lupinova[1], R.V. Denisov[1], A.O. Stepanenko[2], E.A. Mironets[3], V.D. Chivanov[3], A.V. Kochenko[3], E.I. Zinchenko[3]. **Thermal decomposition of the biogenic calcites** ([1]*Sumy National Agrarian University, Ukraine,* [2]*Sumy State University, Ukraine,* [3]*Institute of Applied Physics, NAS of Ukraine, Sumy,*).
133. **A.Yu. Chobotarov**, Ya.I. Savchuk, K.S. Tsyganenko. **Antifungal activity against plant pathogenic fungi of silver nanoparticles obtained by green synthesis** (*Zabolotny Institute of Microbiology and Virology, NAS of Ukraine, Kyiv*).
134. **N.V. Chuiko**, A.Yu. Chobotarov, Ya.I. Savchuk, I.M. Kurchenko, I.K. Kurdish. ***Azotobacter vinelandii* antifungal activity in the presence of silicon dioxide, palygorskite and bentonite** (*Zabolotny Institute of Microbiology and Virology, NAS of Ukraine, Kyiv*).

135. **E. Dikhtiaruk**[1,2], V. Gun'ko[2], V. Paientko[2], A. Matkovsky[2], S. Alekseev[1], A. Kotliarova[3], O. Kotyk[3]. **PVA/chitosan cryogels filled by lignin: synthesis and properties** (*[1]National Taras Shevchenko University of Kyiv, Ukraine, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [3]Bogomolets Institute of Physiology, NAS of Ukraine, Kyiv*).
136. **A. Gaidai**, P. Vakuliuk, I. Furtat, N. Kunytsia, T. Murlanova, O. Golub. **Adsorption of proteins on nano-silica modified with antimicrobial drugs** (*National University of Kyiv-Mohyla Academy, Ukraine*).
137. **A.P. Golovan**, T.V. Krupska. **The effect of the presence of organic and mineral components in AM1-based composite systems on morphological characteristics of tomato sprouts** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
138. **L. Golovkova**, N. Vlasova, T. Budnyak, V. Tertykh. **Bile acid adsorption on the chitosan-containing silica surface** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
139. **L.K. Japaridze**, Ts.S. Gabelia, E.S. Salukvadze, N.A. Osipova, T.K. Kvernadze, O.G. Lomtadze. **Medical-preventive drug against iron deficiency anemia in animals** (*Petre Melikishvili Institute of Physical and Organic Chemistry, Ivane Javakhishvili Tbilisi State University, Georgia*).
140. **R. Ivannikov**[1], L. Buyun[1], I. Laguta[2], O. Stavinskaya[2]. **Disintegrating dosage forms for prolonged antioxidants release based on silica-gelatine matrix and orchids extracts** (*[1]M.M. Gryshko National Botanic Garden, NAS of Ukraine, Kyiv, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
141. **O. Kazakova**, O. Stavinskaya, I. Laguta. **Effect of quercetin on the swelling behaviour of silica-gelatine matrices for prolonged antioxidants release** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
142. **N.Y. Klymenko**, I.V. Siora, E.A. Novikova, T.V. Krupskaya, V.V. Turov. **Model systems for bioremediation of the water containing the mixture of hydrophilic and hydrophobic silica and bacterial cultures** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
143. **I.K. Kurdish**, A.O. Roy, N.V. Chuiko, I.O. Skorochod, A.Yu. Chobotarov. **Perspective of nanomaterials uses at microbial biotechnology** (*Zabolotny Institute of Microbiology and Virology, NAS of Ukraine, Kyiv*).
144. **N.O. Lipkovska**, V.M. Barvinchenko. **Sorption of natural flavonoids on the nano alumina surface** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
145. **O.V. Markitan**, N.N. Vlasova. **Nano-bio interactions: adsorption of the nucleotides onto nanocrystalline titania surface** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
146. **N.M. Opanaschuk**[1], A.L. Petranovska[1], P.P. Gorbyk[1], N.V. Kusyak[1], N.Y. Lukianova[2], V.F. Chehun[2]. **The investigation into a cytotoxic action of vector magnetic liquids with adsorbed gemcitabine *in vitro*** (*[1]Chuiko Institute of Surface Chemistry NAS of Ukraine, Kyiv, [2]R.E. Kavetsky Institute of Experimental Pathology, Oncology and Radiobiology, NAS of Ukraine, Kyiv*).
147. N.M. Opanashchuk[1], A.L. Petranovska[1], P.P. Gorbyk[1], A.P. Kusyak[1], **O.D. Shcheglov**[2], N.G. Antoniuk[2]. **Synthesis of magnetosensitive nanocomposites with carbon surface** (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]National University of Kyiv-Mohyla Academy, Ukraine*).

148. **I.O. Skorochod**, I.K. Kurdish. **Change of qualitative composition of the phenolic compounds at cultural medium of the *Azotobacter vinelandii* IMV B-7076 at their cultivation with palygorskite nanoparticles** (*Zabolotny Institute of Microbiology and Virology, NAS of Ukraine, Kyiv*).
149. **T.V. Travinskaya**, A.N. Brykova, Y.V. Savelyev. **Natural components based environmentally friendly ionic polyurethanes** (*Institute of Macromolecular Chemistry, NAS of Ukraine, Kyiv*).
150. **V.G. Tsitsishvili**, N.M. Dolaberidze, M.O. Nijaradze, N.A. Mirdzveli, Z.G. Amiridze. **Bactericidal adsorbents obtained by ion exchange modification of natural phillipsite** (*Petre Melikishvili Institute of Physical and Organic Chemistry, Ivane Javakhishvili Tbilisi State University, Georgia*).
151. **H. Yankovych**, M. Václavíková. **Adsorbable organic halogens as wastewater contaminants** (*Institute of Geotechnics, Slovak Academy of Sciences, Košice*).
152. **A. Yanovska**[1], D. Nahornyy[2], V. Ivchenko[3], D. Gusiev[1], S. Bolshanina[1]. **Formation of nanoporous bioactive coatings by anode oxidation method** (*[1]Sumy State University, Ukraine, [2]Institute of Applied Physics, NAS of Ukraine, Sumy, [3]Sumy National Agrarian University, Ukraine*).
153. T.V. Krupskaya, **N.V. Yelahina**, V.V. Turov. **Hydration of alginic acid and the influence of the hydrophobic environment in the presence of hydrochloric acid** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
154. **N. Zhorzholiani**, K. Amirkhanashvili, L. Metreveli, A. Dadianidze, A. Shubitidze, L. Khmaladze. **Synthesis and characterization tetra-acid complexes of anesthetic preparations** (*Petre Melikishvili Institute of Physical and Organic Chemistry, Ivane Javakhishvili Tbilisi State University, Georgia*).

5. Metal-based Biocompatible Nanoparticles: Synthesis and Applications

155. **Yu. Harahuts**, N. Kutsevol, A. Naumenko, P. Virych, O. Boyko, O. Nadtoka. **Aggregation processes in multicomponent nanosystems** (*Taras Shevchenko National University of Kyiv, Ukraine*).
156. **O. Hreshchuk**[1], V. Dzhagan[1], M. Stetsenko[1], Iu. Mukha[2], N. Vityuk[2]. **Design and characterization of SERS substrates** (*[1]V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, Kyiv, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
157. **O. Fedyshyn**[1], Iu. Mukha[2], N. Vityuk[2], A. Khodko[3], M. Malysheva[1], A. Eremenko[2]. **Effects of photoactivation of amino acid tryptophan on silver nanoparticles formation** (*[1]Department of Chemistry, Taras Shevchenko National University of Kyiv, Ukraine, [2]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [3]Institute of Physics, NAS of Ukraine, Kyiv*).
158. **O. Nadtoka**, N. Kutsevol, P. Virych, A. Naumenko. **Silver nanoparticles photogeneration in cross-linked Dextran-graft-Polyacrylamide hydrogels** (*Taras Shevchenko National University of Kyiv, Ukraine*).
159. **O.V. Mykhailenko**, S.R. Petrusenko, Ya.O. Vitushinska, Yu.I. Prylutskyy, D.O. Zavodovskyi, O.O. Mykhailenko, O.Yu. Lagerna. **Design, synthesis and biological properties of C_{60}-lactate complexes** (*Taras Shevchenko National University of Kyiv, Ukraine*).
160. **I.S. Petrik**[1], A.M. Eremenko[1], A.V. Rudenko[2]. **Formation of tryptophan complexes with silver and copper nanoparticles on the surface of tissues with stable bactericidal action** (*[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, [2]Institute of Urology, NAMS of Ukraine, Kyiv*).

161. **F.G. Svensson**, G.A. Seisenbaeva, V.G. Kessler. **Titanium alkoxide complexes as molecular models for surface interaction between drug and sol-gel derived titania nanoparticles for drug delivery** (*Department of Molecular Sciences, Swedish University of Agricultural Sciences, Uppsala*).
162. **P.A. Virych**[1], O.M. Nadtoka[1], N.V. Kutsevol[1], V.M. Krysa[2], B.V. Krysa[2]. **Antimicrobial properties of hydrogels/silver nanoparticles composites for surgical use** (*[1]Taras Shevchenko National University of Kyiv, [2]Faculty of Pharmacy, Ivano-Frankivsk National Medical University, Ukraine*).
163. **T.B. Zheltonozhskaya**[1], N.M. Permyakova[1], T.A. Kondratiuk[2], T.V. Beregova[2], V.V. Klepko[1], B.S. Melnik[3]. **The biological effect of stabilized silver nanoparticles on pathogenic hospital microorganisms, the healing process of open wounds and the growth of winter wheat** (*[1]Institute of Macromolecular Chemistry, NAS of Ukraine, Kyiv, [2]Taras Shevchenko National University of Kyiv, Institute of Biology and Medicine, Ukraine, [3]Scientific-Reseach Center of "Kernel", Kyiv, Ukraine*).

The 1932 Nobel Prize in Chemistry: Irving Langmuir

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The very first Nobel Prize in Chemistry awarded for discoveries in surface chemistry was awarded in 1932 to Irving Langmuir. He was nominated five times in physics, of which two times by Niels Bohr (Nobel Prize in Physics 1922). Langmuir was also nominated several times in chemistry, and he received two nominations in 1932, the year he was awarded the Nobel Prize in Chemistry.

In my talk, I will describe the arguments used in the nominations, and the deliberations by the Nobel Committee for Chemistry.

Effects of synthesized polyelectrolytes on structure formation in soil dispersions

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One of the main problems of modern applied colloid chemistry is the study of structure formation processes in dispersed systems under the influence of surface-active substances (SAS) and polyelectrolytes (PE). Numerous scientific studies have unequivocally shown the fundamental possibility of converting structureless soils in ostrate structure using SAS and PE.

The purpose of the work is to study the possibility of using copolymers of maleic acid with acrylamide as structuring agents for the mineral dispersions.

The viscosity measurement of the filtrates before and after adsorption of polyelectrolyte (PE) on the surface of the solid phase in suspension can be used to determine the value of its adsorption. The adsorption of MKAA-5-H in the concentration range of 0.01-0.50% is less compare to MAA-5-K and MAAG-5-K due to the presence of carboxyl groups that are weakly dissociated leading to more minimized state of macromolecules (the counter ions are hydrogen ions). The MAA-5-K polyelectrolyte was obtained by neutralization with caustic potassium where the counter ions of carboxylate groups are potassium ions. Due to the better ionization of the carboxylate groups, the number of negatively charged polyions in MAA-5-K is significantly higher than in MCAA-5-H providing a less curved conformation of the PE macromolecules.

The presence in the composition of PE of positively charged functional groups in sufficient quantity leads to an increase in the amount of adsorption of its macromolecules on the soil, which is associated with a decrease in the ion cloud around the functional groups and compression of the outer diffuse part of the electrical double layer of soil particles.

The isotherms of PE adsorption on soils correspond to Langmuir isotherms indicating the molecular nature of adsorption. At low concentrations of PE (0.01-0.05 g/l) under conditions of intensive growth of the value of adsorption, the binding of particles into aggregates proceeds via an adsorption mechanism. At high concentrations, the structured framework should be called adhesive formation, and the transition from the adsorption to the adhesive mechanism of structure formation occurs gradually.

The adsorption value of MKAA-5-H and MAA-5-K on solid surface is less due to the low degree of ionization and the number of ionizable functional groups compare to MAAG-5-K.

Synthesis and properties of solid solutions of ytterbiy-ittrium ferro garnets

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The development of the component basis for microwave electronics is in two main directions. The first is connected with the development of constructive solutions of ferrite devices that provide the technical and operational requirements set for the systems. The second with the development of technological foundations and methods for improving the component basis for microwave systems.

Widely used as substrates for microstrip devices of microwave electronics found polycrystalline Yttrium ferro-grabs of different compositions. Properties such as glow and ferrimagnetism make grenades interesting for technological applications, lead to the possibility of adjusting the properties of grenades by creating different types of solid solutions. The range of substances and methods of synthesis of materials for this purpose are constantly expanded. Significant interest is solid solutions of ytterbium-yttrium ferrite with a grenade structure. which includes a rare earth compound.

The highly effective methods of synthesis of nanocrystals $(Y_{1-x}Yb_x)_3Fe_5O_{12}$ have been developed. The method of chemical deposition, which includes the stage of recrystallization, uses microwave radiation.

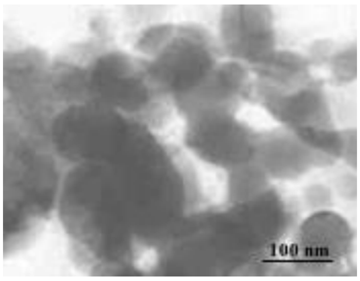

Fig. TEM microphotography of nanoparticles

Synthesized single-domain nanoparticles of solid solutions of ytterbiy-ittrium ferro garnets (Fig.). Their crystalline structure, surface morphology and magnetic properties are investigated by methods of X-ray diffraction analysis, translucent electron microscopy and vibration magnetometry. The dependences of the magnetization of saturation and the coercivity of nanoparticle ensembles on the concentration of components of solid solutions are determined.

Wetting properties of liquid on nanostructured surfaces in coarse-grain approach

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Insight regarding a liquid wetting of a solid surface has important practical appliance and technological relevance in chemical industry, material science, *etc*. Particularly, it is crucially important for performing proper surface functionalization of the nanostructured surfaces. Thus, understanding of interfacial phenomena at the nanoscale is certainly essential.

Molecular dynamics is an efficient tool for study of phenomena arising at the interface between different species. The main advantages of this approach are based on the possibilities of interface reconstructing at the atomistic level. However, significant computational resources required for simulations are strong drawbacks of its successive application. From this point of view, coarse-grained molecular dynamics technique is started to be more and more widely used. Nevertheless, the chosen of concrete coarse-grained model is dependent on the physics of the considered system. Consequently, additional investigation of interactions between atoms of different sorts and phases is significant to reproduce well properties of the system.

Thus, we considered a nanoscale water droplet located on the structured solid surface. For representation of a water molecule, we use one-site coarse-grained electrically-based ELBA model [1]. The wetting states of the droplet depending on the features of surface structuration (roughness and morphology) were studied in detail. With the variation of the parameters of interactional potential, we considered applicability of Wenzel's and Cassie–Baxter models for wetting angle [2].

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Comparative investigation of scattering of conduction electrons on adsorbed submonolayers of hydrogen and deuterium

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Among the variety of phenomena associated with hydrogen adsorption, isotopic effects play a special role. In particular, the two-fold difference of the masses of protium (H) and deuterium (D) is reflected in different binding energies of the adsorbates, their sticking probabilities [1], and surface diffusion rates [2].

We present results of a comparative study of the conduction electrons scattering on H and D adatoms adsorbed on a 100 μm-single crystal Mo (110) plate. The experiment, performed by the static skin effect technique [3] at different submonolayer coverages of the isotopes, reveals the qualitative similarity of magnetoresistance (MS) behavior, but clear difference of the absolute MR values (Fig.).

A possible reason of the isotope effect is discussed in terms of numerical simulations of the electron-phonon interaction.

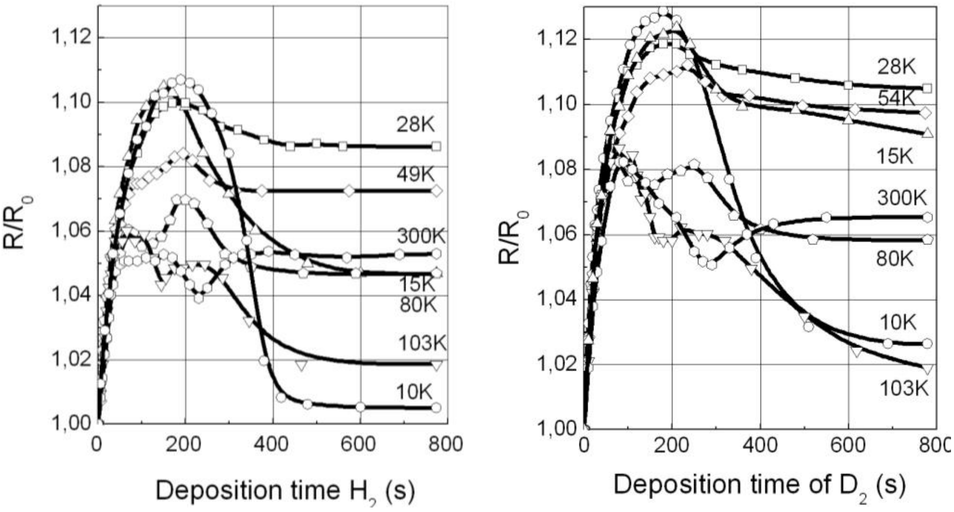

Fig. Relative MS change of the Mo (110) plate during submonolayer adsorption of H (left) and D (right) at different substrate temperatures. The MS measurements were carried out at T = 4.2 K, R_0 is the MS of the atomically clean Mo (110) plate

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Influence of endogenous metabolism of yeast *Saccharomyces cerevisiae* in magnetite-based magnetic fluid

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Much attention in the modern world is paid to nanotechnology with the use of magnetically modified living cells while maintaining their viability. Multifunctional magnetic nanoparticles are widely used in biomedicine, chemistry, physics, and other areas of science, but many issues remain unresolved.

The vital activity of *Saccharomyces cerevisiae* yeast cells (Saf Levure) was studied in magnetite-based magnetic fluid stabilized with sodium oleate in concentration ranges of 0-1% by weight. The kinetics of the process of thermal release of cellular organisms during the enzymatic process under anaerobic conditions of endogenous metabolism was studied. A differential microcalorimeter (DMC) was used in the isothermal regime (295 ± 0.5 K). The sensitivity of the DMC on the heat flux was 10^{-6} W.

Aqueous colloids of nanocomposite particles of magnetite / oleate sodium composition were manufactured. Magnetosensitive colloidal systems were synthesized on the base of magnetite stabilized with sodium oleate modified with polyethylene glycol (PEG-2000). The colloids were described as polydispersion consisting of particles ranging in size from 2 to 22 nm (the maximum of the distribution ~ 7.5 nm) by X-ray analysis, X-ray photoelectron spectroscopy, and transmission electron microscopy.

With an increase in the magnetite concentration, a decrease in the vital activity of cell organisms is observed. At the same time, the presence of magnetic fluid on the stage of hydration of the cellular organism does not have a noticeable effect. Within the studied concentrations, a slight decrease in the vital activity of cell organisms is not accompanied by its complete cessation. In contradistinction to, as for the previously studied CuI nanoparticles, their clearly bactericidal properties are manifested.

Effect of oxygen adsorption on the thermal stability of beryllium nanolayers on the Mo (110) surface

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The interaction of oxygen with beryllium surfaces is of great interest for nuclear, spacecraft and other technologies due to the peculiar character of the interaction of Be with photons and neutrons. In particular, beryllium layers are suggested for the first wall of fusion reactors, for UV-mirrors *etc*. Moreover, beryllium oxide is a promising 2D graphene-like material with unique properties. Recently, it was shown that 2D honeycomb BeO monolayer formed on the Mo (112) surface [1,2].

In the present work, the adsorption of the Be atoms on the Mo (110) surface and the coadsorption of Be with O_2 molecules were investigated by means of experimental studies and first-principles simulation. The experiment was carried out in the ultra-high vacuum chamber (10^{-11} Torr) using the following methods: temperature-programmed desorption (TPD) with mass spectrometric detection (QMS); molecular beam (MB); isothermal desorption (ID); Auger electron spectroscopy (AES). Therefore, we could investigate the adsorption-desorption processes comprehensively, "*in situ*". The calculations were performed on the basis of the density functional theory (DFT) with periodic boundary conditions (ABINIT package).

We investigated electronic properties and thermal stability of Be/Mo, BeO/Mo, and O/Mo adsorption systems. BeO was found to form during adsorption and dissociation of O_2 molecules on the Be/Mo (110) surface. Long-term annealing of Be/Mo(110) at $T = 800–1100$ K in vacuum 10^{-10} Torr, apparently, led to the formation of the surface alloy Be-Mo, which decayed at $T = 1550$ K. It has been shown that the products of desorption from the BeO/Mo (110) adsorption system are beryllium and oxygen atoms. BeO dissociates on the Mo surface at $T > 1700$ K. It is characterized by higher energy of binding with the Mo surface than that which is characteristic of metallic Be ($T \approx 1260$ K). The binding energies of the Be, O atoms and BeO nanostructures were calculated. Hexagonal BeO nanostructures are determined to form on the Mo (110) surface. The stability and electronic properties of the BeO nanostructures on the Mo (110) are discussed.

It has been concluded that the overlayer containing Be can acquire higher thermal stability due to oxidation of beryllium.

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A method for studies of the electrophysical properties of the electrical double layer in nanofluids

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The electrical properties of suspensions of nanoparticles (nanofluids) are dramatically affected by the features of the particle-liquid interface and those of the adjacent electrical double layer (EDL) [1]. Reliable interpretation of experimental data is seriously hindered by the lack of consistent electrodynamic homogenization theories for many-particle systems with complex microstructure.

In this report we:

1) present a new approach to the problem which is based on our recent results for the effective electric conductivity σ for the model of hard-core–penetrable-shell spheres [2, 3]. These were obtained within the so-called compact group approach (see, for instance, [4]). The main equation for σ reads

$$(1-\varphi(c,\delta))\frac{\sigma_0-\sigma}{2\sigma+\sigma_0}+c\,\frac{\sigma_1-\sigma}{2\sigma+\sigma_1}+\int_0^{\delta}du\,\frac{\partial\varphi(c,u)}{\partial u}\,\frac{\sigma_2(u)-\sigma}{2\sigma+\sigma_2(u)}=0\,. \qquad (1)$$

Here: c and $\varphi(c,\delta)$ are the volume concentrations of hard cores (associated with particles) and spheres (particles and the adjacent EDLs), respectively; δ is the relative shell thickness; σ_0 and σ_1 are the conductivities of the carrying liquid and the particle, respectively; and $\sigma_2(u)$ is the conductivity distribution in the shell as a function of the relative distance u from the point of interest to the center of the particle.

2) apply this approach to experimental data for σ of nanofluids based on water solutions of KCl and HCl with high ionic strengths to estimate the electric charge of the suspended nanoparticles, parameters of their EDLs, and the conductivity distribution in them. The processing results demonstrate the adequacy of the Dukhin solution for the electric potential distribution in thin EDLs. The role of the surface conductivity of the particles is discussed as well.

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Functionalized silica-coated lanthanide-doped $NaYF_4$ upconversion nanocrystals

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Upconversion nanoparticles (UCNPs) are a new generation fluorophores which absorb two or more photons and emit shorter wavelength than the excitation (anti-Stokes type emission). Due to this property, UCNPs have been beneficially used in biomedicine for cancer therapy, fluorescence imaging, bio-detection and drug delivery. Upconversion process highly depends on the concentration of doped rare-earth metal ions which are activators and sensitizers in host lattice [1-3]. One of the essential requirements to make use of nanocrystals in biological environments is that the nanoparticles should have a hydrophilic surface.

In order to find out upconversion emission dependence on surface properties the lanthanide-doped upconverting $NaYF_4$ nanoparticles with different functional groups on surface were synthesized. In this research α- and β-phase $NaYF_4$ upconverting nanoparticles doped with Yb^{3+} (20%) and various concentrations of Er^{3+} (0÷5%) were synthesized via thermal decomposition method at 300-330°C in oleic acid and 1-octadecene. Upconverting nanoparticles were modified via Stöber or microemulsion methods using NaYF4:Yb^{3+} (20%), Er^{3+} (2%), tetraethyl orthosilicate (TEOS) or/and (3-aminopropyl)triethoxysilane (APTES), ammonia and cyclohexane. Synthesized materials were characterized by X-ray powder diffraction (XRD), infrared spectroscopy (IR), scanning electron spectroscopy, dynamic light scattering (DLS); upconversion (UC) luminescence properties were measured with Edinburgh Instruments FLS980 (980 nm excitation) spectrophotometer. The smallest nanoparticles (20-35 nm) can be achieved modifying nanoparticles via Stöber method.

Acknowledgements
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Changes in thermal characteristics of Si, SiO_2 and porous silicon under the influence of temperature

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Now scientific and practical interest is growing in systems based on porous silicon materials that would ensure the application of the semiconductor in creating a new generation of opto-, micro- and nano electronic devices. In the goal of this paper, the features of changes in the characteristics of Si, SiO_2 and porous silicon (PS) containing in nanocrystal surrounded by SiO_2 matrix caused by intense thermal radiation have been experimentally studied.

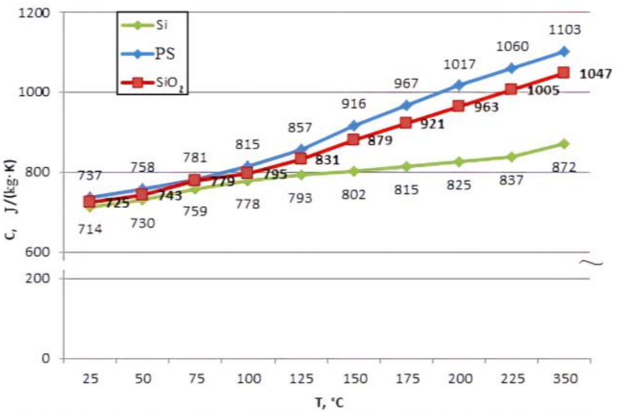

Fig. 1. Temperature dependence of the heat capacity of Si, SiO_2 and PS

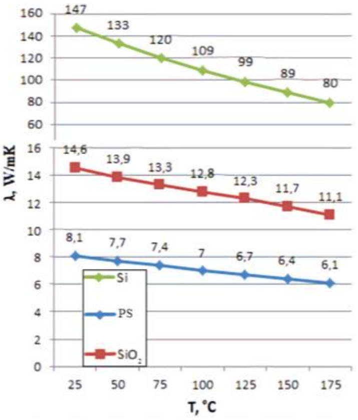

Fig. 2. Temperature dependence of thermal conductivity of Si, SiO_2 and PS

In this paper, it is shown that the heat capacity of Si, SiO_2 and porous silicon increases with increasing temperature (Fig. 1), and the thermal conductivity of the materials decreases with increasing temperature (Fig. 2). Thus, in materials Si, SiO_2 and porous silicon, a highly dispersed structure is formed that contains pores with sizes of 50 ÷ 500Å [1]. At the same time, this trend is observed at a fixed temperature for the materials. These data indicate that the pore size decreases with increasing of the temperature.

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Active carbon from agricultural wastes for adsorption of organic pollutants

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Agricultural waste materials (pistachio shells and strawberry seeds) were used for preparation of active carbons by two various methods. Chemical activation using acetic acid and physical activation with gaseous agents (carbon dioxide, steam) were chosen as mild and environmentally friendly ones. The effect of type of raw material, temperature and activation agent on the porous structure characteristics of the materials was discussed applying nitrogen adsorption/desorption isotherms. Furthermore, XPS, SEM, TEM and thermal analysis were employed to determine the physicochemical properties of the adsorbents. Selection of a raw material and optimization of conditions of the synthesis process allowed to obtain cheap sorbents with a targeted distribution of pores enabling effective adsorption of the model organic pollutants from the multicomponent systems. Adsorption effectiveness (capacity and rate) of the chosen active carbons was estimated for crystal violet (CV), 4-chloro-2-methyphenoxyacetic acid (MCPA), 2,4-dichlorophenoxyacetic acid (2,4-D) in one- or two-component systems. The relatively high rate and adsorption capacity for the dye and herbicides evidence that these cheap sorbents can be considered valuable for treatment of organic pollutants from aqueous solution. The model of adsorption on energetically heterogeneous solids was utilized for isotherm analysis (Generalized Langmuir isotherm equation – GL). The measured concentration *vs*. time profiles for the adsorption systems were analyzed using the Elovich, pseudo first-order (PFOE), pseudo second-order (PSOE), mixed 1.2-order (MOE) equations as well as the multi-exponential equation (m-exp). The applicability of the kinetic equations was evaluated with regard to fitting quality and compatibility with the adsorption process mechanism.

Acknowledgements

The research leading to these results has received funding from the Project: MINIATURA1 -National Science Centre (NCN) of Poland “Active carbons from agricultural wastes for adsorption of environmental pollutions.” Project number: 2017/01/X/ST5/01369.

Studies of thermal behavior of adsorbed organic pollutants on activated carbon

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Pollution of surface and ground waters with toxic organic and inorganic compounds is dangerous because of their potential health hazards. Pesticides are group of toxic compounds that may pollute water due to their extensive application in agriculture. Phenoxyalkanoic acid derivatives are widely used as herbicides and synthetic plant growth regulators. (4-CPA) 4-chlorophenoxyacetic acid, (CFA) clofibric acid, (2,4-D) 2,4-dichlorophenoxyacetic acid, (MCPA) 4-chloro-2-methylphenoxyacetic acid, (MCPP) mecoprop are typical substances used for those purposes. Due to their wide application in agriculture, high solubility in water, phenoxyalkanoic acids easily enter surface or ground waters through natural drainage or infiltration. The toxicity of phenoxyalkanoic acids and their degradation products (chlorophenols) makes the contamination caused by these chemical substances a potential environmental hazard. Activated carbon is the most effective and widely used adsorbent for removal of organic pesticides from aqueous solutions owing to its highly developed structural properties such as specific surface area, porosity and surface chemistry.

The aim of this work was to analyze thermal behavior of adsorbed MCPA pesticide active carbon from agricultural wastes using TG/DTA coupled with mass spectrometry (TG/DTA-MS) and infrared spectroscopy (TG/DTA-IR) techniques. The study of thermal decomposition of chosen systems allowed to get information on influence of accompanying compounds on thermal stability adsorbed MCPA on activated carbon in the multicomponent system. The structure characteristics of the carbon were obtained from the low-temperature adsorption/desorption isotherms of nitrogen and imaging by high-resolution transmission electron microscopy (HRTEM). The surface characteristics in solution were analyzed by using potentiometric titration method.

Acknowledgements

The research leading to these results has received funding from the Project: MINIATURA1 -National Science Centre (NCN) of Poland “Active carbons from agricultural wastes for adsorption of environmental pollutions.” Project number: 2017/01/X/ST5/01369.

The synthesis and adsorption-structure characteristics of carbon-kaolinite composites

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Two series of carbon-inorganic composites were synthesized via carbonization (at 800 °C, Ar atmosphere) of resorcinol-formaldehyde polymers (RFR) mixed with kaolinite. Synthesized samples differ in the mass resorcinol-to-formalin ratio. The samples of the first series (labeled as C1, C2, and C3) were prepared by simultaneous mixing of bentonite, resorcinol, formaldehyde, and distilled water of appropriative amounts. The polymer content in the C1, C2 and C3 samples was 57.6, 47.7, and 34.9 wt. %, respectively. The second series (C4, C5, and C6 samples) was prepared by prolonged exposure of kaolinite in a solution of polymer components at the content of 56.1, 45.1, and 33.4 wt. %, respectively. The structure and morphology of the nanocomposites were characterized using low-temperature nitrogen adsorption (Fig.), TG/DTG, DSC, XRD, SAXS, and Raman spectroscopy. According to the XRD data, the penetration of organic components into the spaces between packets of kaolinite layers took place during the synthesis. Two stages of thermo-oxidative decomposition of polymer at 300 and 460-500 °C were registered using TG/DTG. The specific surface area (S_{BET}) of carbonized samples varied from 98 to 245 m^2/g (S_{BET}= 9 m^2/g for initial kaolinite). The prepared composites are characterized by different particle sizes, shape, and degree of graphitization.

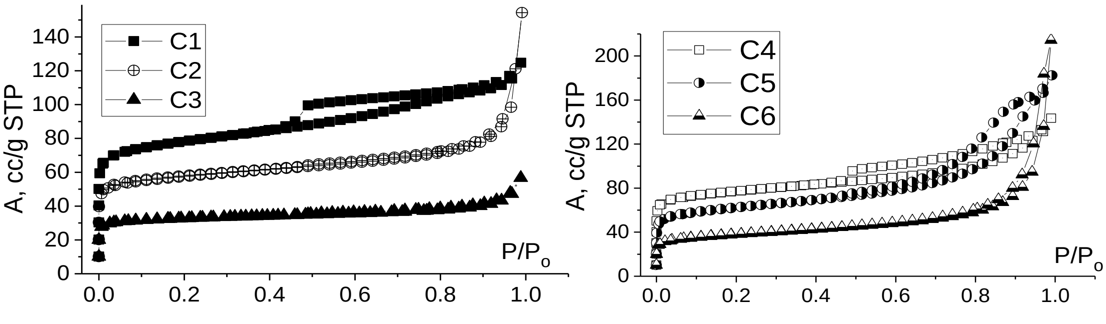

Fig. Nitrogen adsorption/desorption isotherms for carbonized composites

Thus, the results show that the textural and morphological characteristics of the nanocomposites strongly depend on the synthesis method.

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Biodegradable composite materials on base of cellulose acetate

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Cellulose esters represent a class of polymers that has the potential to participate in the carbon cycle via decomposition of the resulting cellulose and organic acids. Cellulose acetate is currently used in high volume applications ranging from fiber, to film, to thermoplastics. It has the physical properties and relatively low material cost that have excluded other biodegradable polymers from being widely accepted in the market place. Organic/inorganic polymer hybrids are a rapidly growing area of research [1]. There are several routes to prepare hybrid materials, but one of the most common method is sol-gel technique generating inorganic phase within organic polymer matrix. This process includes hydrolysis of the precursor (metal alkoxide) followed by condensation reactions of the resulting hydroxyl groups. Considering the nature of the interface between the organic and inorganic phases, hybrid materials can be prepared. A preparation stages of hybrids was as follows [2].

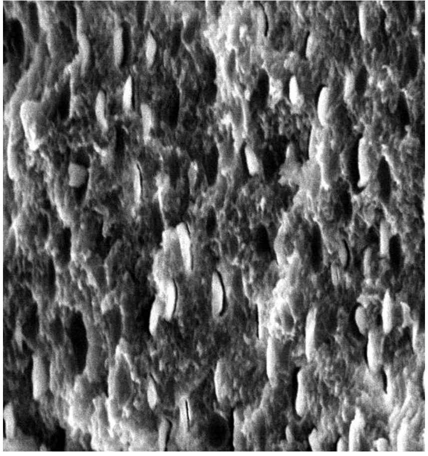

Fig. SEM image of organic-inorganic hybrid

Cellulose acetate butyrate powder was placed in a beaker and dissolved in acetone. Plasticizer (propylene glycol) and TEOS were then added and mixed vigorously. To this solution catalytic amount of HCl (0.1 M) was added to initiate the sol-gel process. The solution was cast in PTFE dish and left exposed to atmospheric conditions followed by drying in an oven at 60°C for 6 hours to ensure complete solvent evaporation. The prepared films were characterized by DTA, X-ray diffraction, IR-spectroscopy, and scanning electron microscopy (SEM) (Fig.). Mechanical properties were investigated using a universal tensile machine (RMI-5).

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Modification of silica gel with tetraphosphorylated calix[4]arenes and examination of Eu(III) sorption

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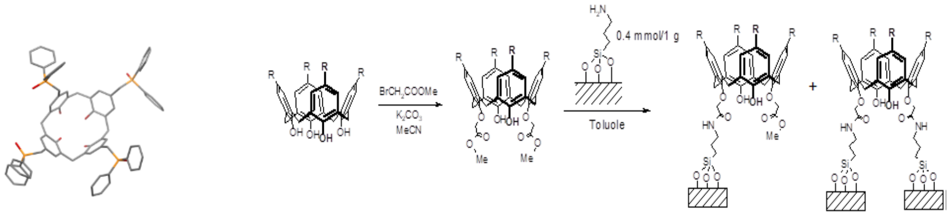
The upper rim phosphorylated calixarenes bearing reactive groups at the lower rim of macrocycle are used for modification of organic and inorganic porous materials. Due to presence of the P=O binding groups at their surface the modified material effectively and selectively adsorbs actinides and lanthanides from water solutions [1,2].

In this paper we present synthesis of the cone-shaped calix[4]arenes, modified at the upper rim of the macrocycle with metal-coordinating phosphonate and phosphine oxide groups. Simultaneously, at the lower rim, these calixarenes contain methoxycarbonylmethoxy groups that react with amino groups on the silica gel surface. The reaction is supposed to be the nucleophilic substitution of methanol and the formation of the amide bonds.



R= $CH_2P(O)Ph_2$, $CH_2P(O)(OPr^i)_2$

The structures of the synthesized phosphorylated calixarenes were investigated by X-ray diffraction analysis and NMR spectroscopy methods. The sorbents obtained are monodisperse with an average particle size of 50-100 microns. In the process of covalent fixation of the calixarenes on the surface, the surface morphology and dispersion of the silica gel particles are maintained.

It was also shown that silica gels, modified by the phosphorylated calixarenes effectively adsorb europium from aqueous solutions of nitric acid at pH 5-7. The initial segments of the adsorbtion isotherm are well described by the Langmuir model.

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Synthesis O-*g*-C_3N_4/TiO_2 rutile composite material for photocatalytic application

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For efficient light utilization, fabrication and photocatalytic applications of *g*-C_3N_4/TiO_2 composite materials have attracted much attention [1]. However, both pristine *g*-C_3N_4 and *g*-C_3N_4/TiO_2 composite exhibits photoactivity in the visible spectrum with limited utilization of solar energy (with wavelength below 460 nm). It is found that the doping of carbon nitride by oxygen significantly improves its photocatalytic properties. Therefore, to improve the photocatalytic activity of semiconductor photocatalyst, the coupling O-doped *g*-C_3N_4 (O-*g*-C_3N_4) with rutile TiO_2 is a good strategy. As O-doped *g*-C_3N_4, new composite material – O-*g*-C_3N_4/TiO_2 was synthesized by gas phase method under the special reactionary conditions of the pyrolysis of melamine [2-3]. Deposition of O-*g*-C_3N_4 (~6% O) on the rutile nanopowder particles is confirmed by IR (Fig., *b*), XPS, XRD (Fig., *a*) methods. As a result, both O-*g*-C_3N_4 and O-*g*-C_3N_4/TiO_2 photoactivity boundary in the visible spectrum expands to the whole visible light region and the band gaps of both products is determined to be less than 2.12 and 2.28 eV, respectively (Fig., *d*). Constructing heterojunction structures of TiO_2 and O-*g*-C_3N_4 may be used as a cost-effective way to avoid the drawbacks of each component and realize a synergic effect in promoting the efficient generation and separation of charge carriers, thus boosting the photocatalytic activity.

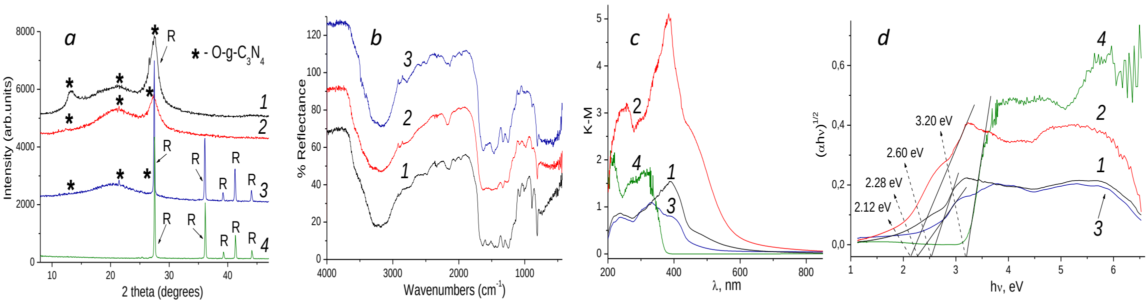

Fig. XRD pattern (*a*), IR (*b*), UV−Vis DRS (*c*) spectra and estimation of band gap energies (*d*) of: *1*– pristine *g*-C_3N_4, *2* – O-*g*-C_3N_4, *3* – *g*-C_3N_4/TiO_2 composite; *4* – pristine rutile TiO_2

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Optical properties of carbon nitride oxide (*g*-C_3N_4)O and O-doped carbon nitride O-*g*-C_3N_4 as perspective photocatalytic materials

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Graphitic carbon nitride (*g*-C_3N_4) has been shown to have huge potential in photo-/electrocatalytic hydrogen generation. However, the ~2.7 eV bandgap of *g*-C_3N_4 make it only utilize the solar light with wavelength below 460 nm. Thus, in order to further enhance the light harvesting ability of *g*-C_3N_4, various bandgap engineering strategies, including doping by oxygen are used. For various kinds of photochemistry-related applications of oxygen-doped carbon nitride (O-*g*-C_3N_4) (4-7% O) and new substance with more oxygen content - carbon nitride oxide (*g*-C_3N_4)O (16% O) [1-3] are decisive the optical properties, including UV/Vis absorption. As a result, the O-*g*-C_3N_4 and (*g*-C_3N_4)O photoactivity boundary in the visible spectrum expands from 460 to 700 and 800 nm (but also adds a shoulder on the absorption edge to further extend the absorption to ~1000 nm) respectively (Fig., *a*, *c*). It is assumed that the absorption spectrum of doped carbon nitride extends to the whole visible light region, possibly due to excitation into the lower energy defect states [4]. As a result, the bandgap of oxidized carbon nitride is determined to be less than 2.10 eV with a sub-gap of less than 1.10 eV corresponding to the absorption edge of the add-on shoulder (Fig., *b*, *d*). In such case, carbon nitride oxide (*g*-C_3N_4)O would absorb more visible light than both *g*-C_3N_4 and O-*g*-C_3N_4, there by generating more charges, which contributed to the improvement in the photoactivity of the catalysts.

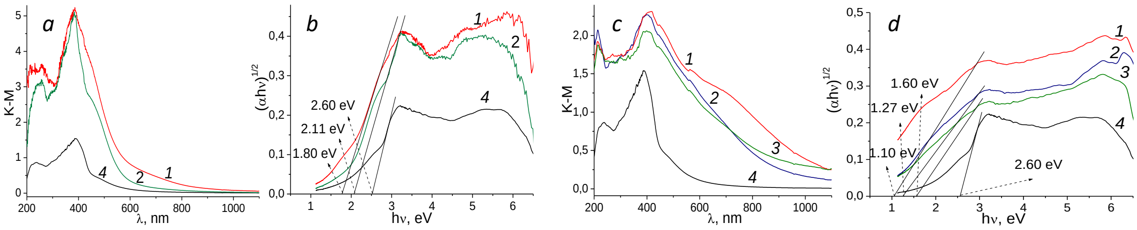

Fig. UV–vis DRS spectra and estimation of band gap energies of O-*g*-C_3N_4 (*a*, *b*), (*g*-C_3N_4)O (*c*, *d*), synthesized from: *1*– urea/cyanuric acid mixture, *2* – urea, *3* – melamine; *4* – pristine *g*-C_3N_4

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Preparation of *g*-C_3N_4/TiO_2 binary films on Ti surface by CVD approach for hydrogen evolution photoelectrodes

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Photocatalytic electrochemical converting water to environmentally friendly hydrogen fuel is one of the most promising clean energy technologies, using renewable energy such as solar energy. Titanium dioxide is one of the most common photoanode materials, but the photocatalytic activity of TiO_2 is greatly limited by its wide bandgap of 3.2 eV. Recently, graphite-like carbon nitride, as a metal-free polymeric semiconductor with inherent chemical and thermal stability, and a moderate bandgap of 2.7 eV, has generated a lot of interest as photoelectrode material for the evolution of hydrogen from water in visible light. In this work, we introduce a facile procedure to obtaining of *g*-C_3N_4/TiO_2 binary composite thin films on titanium foil substrate (Fig., *a*) by one-step CVD approach using urea as precursor. To produce partially oxidized product (TiO_2) on the Ti surface we carried out the pyrolysis of precursor at the presence of a fixed volume of air (under air atmosphere) [1, 2]. The *g*-C_3N_4/TiO_2 films were analyzed by XPS, XRD (Fig., *b*). and IR spectroscopy (Fig., *d*). It was found that the visible-light-induced photodegradation of methylene blue was remarkably increased upon coupling TiO_2 with *g*-C_3N_4. The enhanced catalytic efficiency could be mainly attributed to the well-matched band gap structure with heterojunction interfaceand favorable optical property [3]. The facile deposition method can be promising for the fabrication of efficient and low-cost photoelectrodes based on *g*-C_3N_4/TiO_2 composite films.

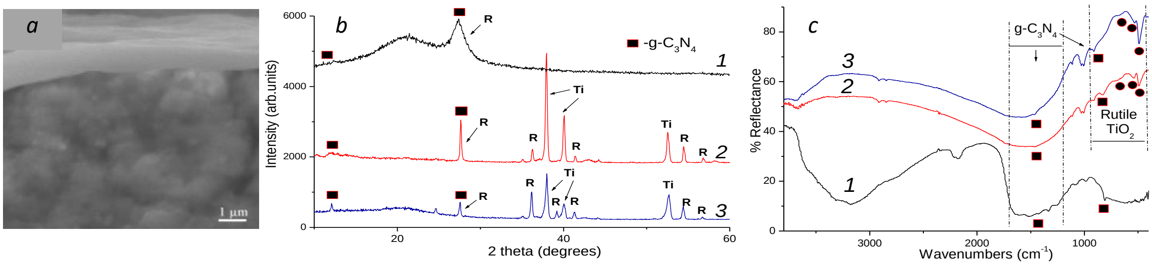

Fig. SEM image of the edge *g*-C_3N_4/TiO_2 film (*a*), XRD (*b*) and IR spectra (*c*) of: *1* – *g*-C_3N_4 and *4* – TiO_2 powders, *2, 3* – *g*-C_3N_4/TiO_2 films obtained at 550°C for 1 and 1.5 h, respectively

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Removal of arsenic(V) from contaminated water with palygorskite supported hydrated Fe(III) oxides

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Heavy metal pollution is an environmental problem that has harmful effect on aquatic environment. Arsenic (As) is a toxic trace element found in groundwater due to natural and industrial processes. As(III) is more toxic and more prone to migration than As(V), but the last one is the most stable form.

The creation of sorbents based on natural aluminosilicates by modifying their surface makes it possible to achieve sufficiently high structural and absorption characteristics. Chemical modification of the surface of layered silicates, in particular hydrated Fe(III) oxide, to improve their sorption properties is promising.

Hydrated Fe(III) oxides have large surface area, strong adsorptive properties, high adsorptive capacity, and low cost make that their an attractive material for removal of both cationic and anionic impurities from wastewater.

The purpose of this work was to obtain a surface-modified silicate material based on palygorskite and ferrihydrite also to study the physicochemical features for the removal of arsenic(V) from contaminated water using a chemically modified sorbent.

To obtain a composite sorbent based on palygorskite modified with ferrihydrite, the Ca-form of the mineral was carefully placed in a solution of $FeCl_3 \cdot 6H_2O$ during mixed and solution of KOH was added to pH 7 - 8.

According to the duration of the establishment of sorption equilibrium, it can be argued that the As(V) sorption process on all samples increases rapidly and after 1 h of contact, the sorption value remains almost unchanged. Studying the effect of pH on the adsorption process of As(V) ions showed that the magnitude of anion sorption by the obtained composite sample with a deposited layer of ferrihydrite practically does not change in a wide pH range due to the existing excess of adsorption sites. Adsorption of As(V) on natural minerals is strongly pH dependent. As the pH increases, the clay surface becomes more and more negatively charged preventing As(V) anions from approaching the surface and explains the smaller extend of adsorption at higher pH. The value of adsorption for palygorskite modified with ferrihydrite is more than for natural palygorskite, 7.8 mg/g and 0.2 mg/g, relatively.

The removal of As(V) from aqueous environment through adsorption with palygorskite supported hydrated Fe(III) oxides is one of the promising approach due to its high efficiency and low-cost.

Nanocomposites based on PU/PHEMA semi-interpenetrating polymer networks and nanosilica modified by amino acid tryptophane: morphology and properties

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The nanocomposites based on multicomponent polymer matrix consisting of polyurethane, poly(2-hydroxyethyl methacrylate), and nanofillers based on silica with mechanically activated surface and surface modified by amino acid tryptophane (tphn) are synthesized. The structure and properties of the nanocomposites based on PU/PHEMA=83/17 and 63/37 matrices and with nanofiller content 3-15 wt.% tphn were studied.

The investigation of the created nanocomposites by the atomic force microscopy (AFM) have shown that nanoparticles modified by amino acid tryptophane, which incorporated into the polymer matrix with 17% PHEMA, demonstrated the possibility of satisfactory dispersion of tphn particles without their essential aggregation. DSC investigations have shown that presence of nanofiller increases systematically and substantially temperature of glass transition T_g and decreases $\Delta C_{p,norm}$ for PHEMA phase in the nanocomposites with 17% PHEMA. By TSDC studies a weak peak located at around -130 to -120 °C detected which represents $\beta_{sw,PHEMA}$ dielectric relaxation, which is assigned to crankshaft motion of PHEMA side groups with attached water molecules, or it is treated as γ_{PHEMA} relaxation representing rotation of hydroxyethyl groups in the side chain of PHEMA. The temperature position of this relaxation does not change with composition.

Data of dynamic mechanical analysis (DMA) shows substantial changes in the PHEMA tan delta peak due to introducing tphn particles into the semi-IPN17 matrix. Its temperature position and form change non-monotonically with increasing tphn content. On the whole, this peak is displaced, becomes twice broader and sharply asymmetric in the nanocomposites.

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Thermal decomposition of the biogenic calcites

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The spectra of thermal desorption (TDS) of gaseous carbon dioxide (CO_2) emitted from the biocomposite carbonate rostra of belemnite (*Belemnitella Orbigny*) were studied. The main component of rostrum is calcite ($CaCO_3$). It has been shown that the structure of the TDS spectrum of the carbonate roster is a function of the level of dispersity of the components of this biocomposite.

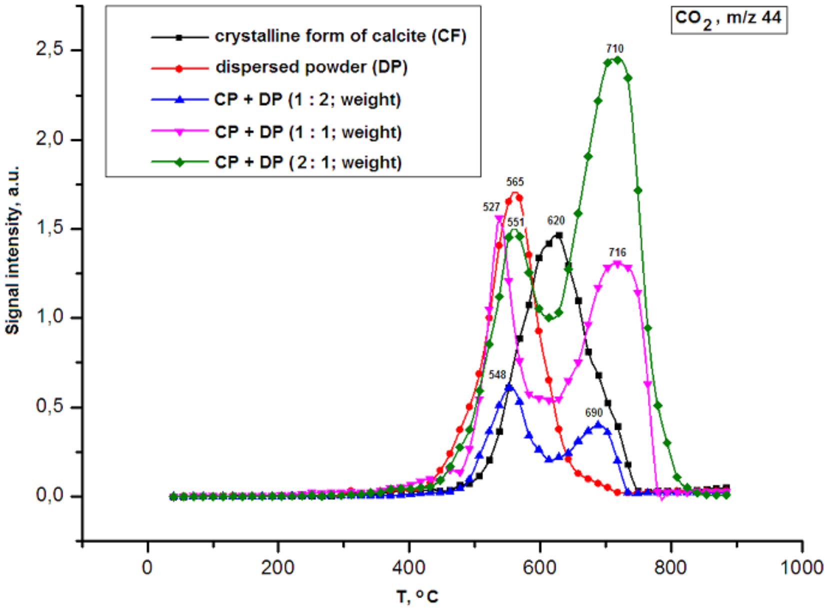

Fig. Thermogram of carbonate rostra of belemnite (*Belemnitella Orbigny*)

An increase in the concentration of ultrafine and micro disperse calcite components in the roster biocomposite leads to a significant change the type of the thermal desorption spectrum of CO_2, which is manifested in the appearance of additional temperature regions of desorption (peaks) and their shift to a region of lower temperatures (Fig.).

The contact angle of nanodroplets

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The contact angle is unambiguously determined at the macroscopic size. However, in the case of nanoscopic size the relatively considerable thickness of the interfacial region, where the density distribution and the component of the pressure tensor are heterogeneous, can cause ambiguity to measure the contact angle. This issue can best be illustrated by taking an example of molecular dynamics simulations of a cylindrical droplet (see Fig.).

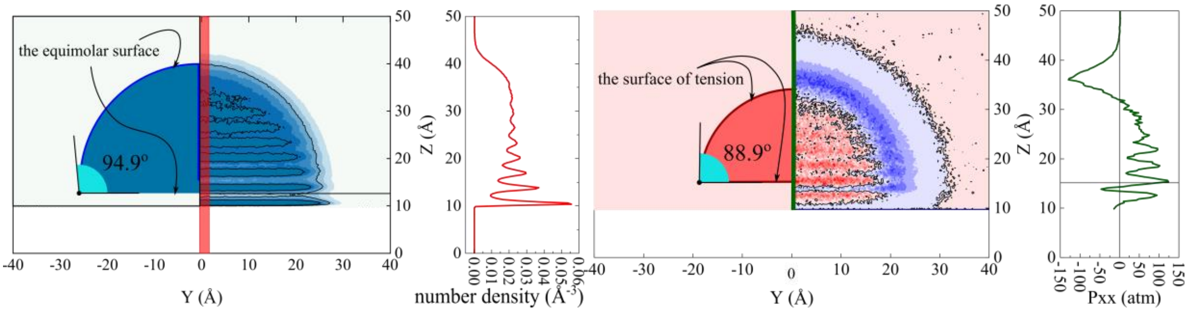

Fig. The contact angle determined as the angle between the equimolar surfaces and as the angle between the surfaces of tension

We propose to consistently use the Gibbs dividing surface method in order to avoid this ambiguity [1]. The essential feature of the Gibbs approach is that the real physical system, which consists of the two adjacent bulk phases that are separated by a finite thickness interface region, is a model reference system, having clearly separated adjacent phases and a certain mathematical dividing surface between them. In addition, the so-called the surface excess, extensive, thermodynamic variables [2] are computed for the dividing surface. With these features of the method, some special case of the dividing surface provides a complete mechanical equivalence of the reference system and the real physical system. This dividing surface is called the surface of tension [3]. That is why we propose that the contact angle should be understood to refer to the dihedral angle between the mathematical dividing surfaces, which are surfaces of tension.

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Use of gold nanoparticles of different sizes, as potential antiviral agents

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Different metal nanoparticles possess broad-spectrum antiviral activity, including gold nanoparticles (Au NPs), that are active AIV, HSV-1, HSV-2, HIV. Albeit the molecular mechanism of such interaction is still unknown.

In this study, we aimed to determine possible antiviral activity of gold nanoparticles against Epstein-Barr virus (EBV) and adenovirus 5 and to define more suitable viral surface for their interaction. Au NPs of different sizes, namely 5 and 20 nm (according to microscopy and dynamic light scattering data). The positions of surface plasmon resonance band maximum in absorption spectra of obtained colloids were located at 510 and 523 nm respectively. The study was conducted with use of transmission electron microscope (TEM) Jeol 1400 (Jeol, Japan) to observe morphological changes of viruses treated with Au NPs and the interaction of nanoparticles with the viral surface. Au NPs of both sizes were used in the final concentration of 9.85 μg/ml. Viruses were incubated in 5 μl of Au NPs colloids for 1 hour during absorption on cupper grid. All samples were stained with 2% uranyl acetate solution.

On TEM photographs of EBV, strong interactions of Au NPs of both sizes with lipid membrane of virus were observed. It was shown, that Au NPs of 5 nm covered all the surface of viral particles and caused a disruption of viral lipid membrane. Whereas in case of Au NPs of 20 nm interact was not so quantitative with viral membrane, on TEM photographs only 1-3 nanoparticles per each viral particle were observed. However, Au NPs of 20 nm also possessed a strong antiviral activity, based on the ability of nanoparticles to cause the disruption of viral lipid membrane. In contrast to EBV, Au NPs of both sizes did not interact with protein capside of adenovirus during 1 hour of incubation. Still a few viruses with disruption were observed in samples. However, extending the incubation time to 2 hours showed a following result: Au NPs of 5 nm caused a significant disruption of viral particles, while Au NPs of 20 nm particles caused an absolute damage of virus. Overall, Au NPs of 5 nm and 20 nm showed a strong virulicidal activity against EBV and adenovirus 5.

Study of glass-reinforced plastic filled by surface modified multiwall carbon nanotubes

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Application of nanosized particles as fillers of polymer binder in order to enhance physico-mechanical characteristics of polymer composites has been actively investigated recently [1-3]. However, the most prevalent use as a reinforcing element is the use of carbon nanotubes (CNT's) as the most effective nanostructures [4,5]. We experimentally studied the multilayer CNT's, which were synthesized by CCVD method by introducing into the epoxy system of LR285-LH286. The effect of modifying the surface of multilayer CNT's by oxygen and nitrogen on the strength characteristics of the fiberglass filled with them was investigated by testing for tension and bending.

It was shown that in epoxide system LR285-LH286 hydrophobic CNT's (outgoing) at introducing into the catalyst polymerization of LH 286, increase the strength with respect to unreinforced CNT's by 48-54%. Oxidized CNT's (200 A·h/kg) introduced into the resin LR285 increase the strength by 59%. The distribution of the filler particles in size, both in the epoxy resin and in the catalyst, depends nonlinearly on their concentration and correlates with the strength characteristics of the composite.

The multilayer CNT's increase the strength of a model laminated fiberglass with a porous core with respect to stretching and bending by 25-35% at low concentrations of CNT's (up to 0.4% by mass). The effect increases with the introduction of CNT's into a less viscous fluid, namely the polymerization catalyst LH286. Modifying the surface of CNT's with oxygen and nitrogen changes their interaction with the epoxy matrix.

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Antifungal activity against plant pathogenic fungi of silver nanoparticles obtained by green synthesis

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In the last decade green synthesis of nanoparticle methods have been introduced and widely used in the production of different types of nanoparticles (NPs). These methods use microorganisms, extracts from various plants, and cell-free extracts of fungi or bacteria. Fungi can produce a wide variety of metal NPs and are good candidates for large scale production because of the simplicity and the cost efficiency of growth on both the laboratory and the industrial scale. From the other hand, the wide spectrum of biocidal activities of NPs obtained by green synthesis gives hope of overcoming the problem of the resistance of infectious disease causative agents to different biocidal drugs and antibiotics.

In this investigation were studied antifungal activity of nanosilver (AgNPs) obtained by green synthesis method using fungal cell-free extracts after *Penicillium* sp. cultivation and silver nitrate solution. The UV-Vis spectrum of the AgNPs solutions were recorded in 420 nm, the morphology and particle sizes investigated by TEM were in the range of 12 – 35 nm. The main aim of present study was the evaluation of the antifungal activity spectrum of AgNPs obtained by green synthesis on a wide set of plant pathogenic fungi. We used 15 strains of test culture from the Culture Collection of IMV of the NAS of Ukraine that are causative agents of plant diseases, including *Alternaria brassicicola, A. tenuissima*, *A. alternata*, *A. longipes*, *Fusarium lactis*, *F. culmorum, F. graminearum*, *F. poae*, *F. moniliforme*, *F. oxysporum*, *F. solani, F. avenaceum, Rhizoctonia solani*, *Botrytis cinerea*, *Bipolaris sorokiniana*. The screening was made by agar well diffusion assay method. 0.2 ml of AgNPs solution was added per well; cultivation was carried out at 26°C. Diameters of the growth inhibition zones of test fungi were measured after 48 hours and the sporulation delay zones were observed during next 5 – 7 days.

The study results showed the antifungal activity of AgNPs against all test cultures except *B. cinerea*. The most sensitive fungi were *R. solani, B. sorokiniana,* and *F. graminearum* with diameters of the growth inhibition zones in the range of 32 – 40 mm; other test cultures had these zones in the range of 17 – 26 mm. All sensitive fungi had the sporulation delay zones with diameters larger by 6 – 10 mm than the inhibition zones.

Antifungal activity of AgNPs obtained by green synthesis method using cell-free extracts of *Penicillium* sp. opens the perspective direction of new eco-friendly biocidal drugs design for plant protection.

Experimental study of composite material on polymeric basis, which possesses antimicrobial activity

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One of the most important directions of modern medicine is the introduction into the medical process of various polymeric materials. Moreover, the modification of these materials greatly extends the area of their application. A promising trend is the saturation of polymeric materials by antimicrobial agents with the possibility of prolonged uniform release of active substances and the creation of the therapeutic concentration in the place of use.

The aim of this work was the experimental study of the effectiveness of a composite material with regulated porosity on a polymeric basis which possesses the antimicrobial properties.

For this purpose, a porous polymer network of poly(2-hydroxyethyl methacrylate) saturated with decamethoxin, chlorhexidine or metronidazole was used. The kinetics of the release of active substances with the measurement of their concentration by spectrophotometric method was examined and the antimicrobial activity of the samples has been studied by agar diffusion test.

As a result, a gradual release of decamethoxin and metronidazole with a maximum degree after 24 and 12 hours, respectively, has been stated; simultaneously 100 % metronidazole release was observed. The highest antimicrobial activity has been found for samples containing decamethoxin, for which the growth inhibition zone was significantly larger than that for other samples and was 18.4 ± 3.0 mm for *Staphylococcus aureus*; 20.4 ± 3.8 mm for *Escherichia coli* and 15.5 ± 2.6 mm for *Pseudomonas aeruginosa*.

Thus, the results of the research confirmed the effectiveness of the developed materials and the feasibility of their further study.

Azotobacter vinelandii antifungal activity in the presence of silicon dioxide, palygorskite and bentonite

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Azotobacter vinelandii IMV B-7076 is a component of the complex bacterial preparation Azogran which increase plants growth, development and yield. Inhibition of phytopathogenic fungi by *Azotobacter* [1] is one of the important properties of these bacteria as part of this preparation. Azogran is made on the basis of bentonite. In natural conditions bacteria can also interact with clay minerals, which are components of many types of soils. In turn, clay minerals are aluminosilicates, which are 70% of silicon oxide and aluminium oxide. The model of individual components of these complex compounds are synthetic materials based on silicon dioxide. Microorganisms can contact with highly dispersed materials that in most cases leads to changes in their physiological and biochemical properties [2]. Therefore it was advisable to investigate *A. vinelandii* IMV B-7076 antifungal activity and the effect of some nanomaterials on it.

It is shown that *A. vinelandii* IMV B-7076 exhibits antagonistic activity toward phytopathogenic fungi *Alternaria alternata* 16861, *Fusarium avenaceum* 50720, *Fusarium moniliforme* 50463, *Fusarium lactis* 50719, *Fusarium oxysporum* 54201, *Fusarium poae* 50704 (the diameter of fungi mycelium growth and spore formation inhibition zone is 14-37 mm), *Bipolaris sorokiniana* 16868 and *Fusarium solani* 50718 (the diameter of zone is 11-13 mm) and does not affect *Fusarium culmorum* 50716 and *Fusarium graminearum* 50662 development. The addition of silicon dioxide, palygorskite and bentonite in the *A. vinelandii* IMV B-7076 cultivation medium in concentrations 0.1, 2.0, 5.0 g/L does not influence on the size of fungi inhibition zone.

These studies helped to understand that the contact with silicon dioxide, palygorskite and the Azogran mineral basis bentonite does not affect the possibility of *A. vinelandii* IMV B-7076 to implement its potential as an antagonist of phytopathogenic fungi.

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Photocatalyst nano TiO_2 / diatomite: the relationship of porous structure, adsorption and photocatalytic activity

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The relationship of the pore structure of the photocatalyst DDT based on nanosized TiO_2 grafted onto the surface of diatomite and its adsorption and photocatalytic activity in relation to the model dye methylene blue (MB) considered in this report in dependence of titania content in the obtained composite. Diatomite D and synthesized TiO_2 also were investigated.

The photocatalyst was prepared via heterogeneous hydrolysis of $TiCl_4$ as a precursor of TiO_2 in the presence of diatomite at room temperature and normal pressure. The obtained product was further washed, dried and calcined at 450°C for anatase phase development. During the synthesis the amount of titania in the products varied from 10 to 75%. Crystal structure, chemical composition and adsorption-structure properties (specific surface area, adsorption pore volume) in nanocomposite and its components were determined with XRD, XPS and EDX analyses and low temperature adsorption of nitrogen.

Adsorption experiments were carried out in a batch mode at adsorbent doze 2g/L, solution pH 7.4, temperature 20°C and initial dye concentration 130 mg/L.

It was shown that with the smallest specific surface area - 36.5 m^2/g, the initial diatomite has the largest adsorption capacity - 74.8 mg MB/g. As the TiO_2 content in products increases, the specific surface area increases up to 147.5 m^2/g, for pure titania, but the adsorption value on the contrary decreases and reaches a minimum for pure titanium dioxide -15.0 mg MB/g. The dependence of photocatalytic activity is more complicated and it is extreme. Diatomite generally does not have photocatalytic properties at all. MB decomposition degree on the DDT products increases at TiO_2 loading up to 20% and reaches maximum -83%. A further increase in the TiO_2 content in samples leads to a decrease in photocatalytic activity up to 65% for product with 75% TiO_2

Obviously, the photoactivity of the synthesized catalysts is determined not only by the value of the specific surface area and adsorption capacity, but also by the size of anatase crystallites, which has been shown to grow with increasing TiO_2 content on the surface of diatomite.

Symmetry rules for Brownian photomotors

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Nanodevices converting non-equilibrium fluctuations to directed motion through the so-called ratchet effect, with the energy supplied by the resonant laser radiation, are referred to as Brownian photomotors [1]. Here we address the necessary symmetry conditions for the ratchet effect to occur [2, 3].

With the symmetry transformations leaving the average photomotor velocity invariant or changing its sign, it is shown that a symmetric substrate (the immovable photomotor part with the symmetric charge distribution) enables the directed motion of a molecule/nanoparticle (the moving photomotor part) only provided the antisymmetric charge distribution fluctuates in it. Switching from a single Brownian particle to an ensemble of randomly oriented particles, it is found that the symmetric substrate provides no directed transport in this collective case, i.e., the ensemble can only diffuse in all directions equiprobably. In contrast, if a substrate has the antisymmetric charge distribution, both single particles and their ensembles can move directly only provided their fluctuating charge distribution is symmetric.

If the time dependence of the charge distribution in particles is described by a *universally symmetric* periodic function (i.e., simultaneously symmetric, antisymmetric, and half-period shift-invariant up to sign), then the ratchet effect is ruled out in the overdamped regime but allowed if the particle inertia is taken into account, provided that the charge distribution in the particle and/or in the substrate are neither symmetric nor antisymmetric.

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S_0-S_1 conical intersections of conjugated compounds

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Based on the AM1-calculated heats of formation for simple conjugated molecules, the conditions for S_0-S_1 state conical intersection (SCI) [1] in the vicinity of the cyanine limit (CL) [2] have been studied. The electronic structural parameters of sparkle-simulated donor-acceptor π-species have been related to the geometry and energy of the state-intersection structures occurring in the corresponding twisted molecules. As shown, twisting and donor-acceptor strength can cause concordant and competing effects on different parameters of state conical intersections.

It is found that the Longuet-Higgins theorem on SCI occurrence [1, 3] is unconditionally valid only for sufficiently small molecules; otherwise, symmetry rules can be violated and, accordingly, the necessary conditions for SCIs are describable only phenomenologically, in terms of certain molecular parameters. Evidently, a SCI can occur in a sufficiently narrow structural range where the prerequisites exist for the S_0-S_1 structural and hence energetic closeness. As far as π-conjugated structures are concerned, this closeness is reached in the vicinity of the CL where the bonds involved in a possible twist are intermediate between double one single. Importantly, there are no universal "critical" values of bond orders or other structural parameters at which twist-induced SCI occurs for different compounds irrespective of their individual constitution. Among other regularities, it is established that the larger the donor-acceptor strength, the closer to 90^0 a SCI occurs, if any. The energy of the SCI structure lowers with increasing donor-acceptor strength. As expected by intuition and confirmed computationally, the twisting and the donor-acceptor strength have an opposite effect on the energy closeness of frontier MOs. On the other hand, they act concordantly in the context of frontier MO localization. It is also demonstrated that the action of a polar environment is in many respects equivalent to the effect of donor-acceptor substituents or an external electric field. Taken altogether, the peculiarities found promise to contribute to the understanding of often observable drastic changes in fluorescence caused by slight structural modifications of polymethine compounds.

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Structure, morphology and antimicrobial properties of silver-containing nanocomposites

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Structural organization, morphology and antimicrobial properties of nanocomposites based on polyelectrolyte complexes pectin–polyethyleneimine and Ag nanoparticles, which formed by the thermochemical reduction methods from interpolyelectrolyte–metal complexes (IMC) pectin–Ag^+–polyethyleneimine have been investigated. It is defined that thermochemical reduction of Ag^+ ions in IMC bulk (while films are heated to the temperature around 100 °C and more) results in formation of nanocomposites. Therefore, according to the wide angle X-ray scattering (WAXS) data we can conclude that the optimal temperature for Ag^+ ions reduction in IMC with further formation of nanocomposite is to be 150°C [1]. Applying TEM, it was found that silver nanoparticles have a fairly even distribution in the polymer matrix with average size of 5.5 nm.

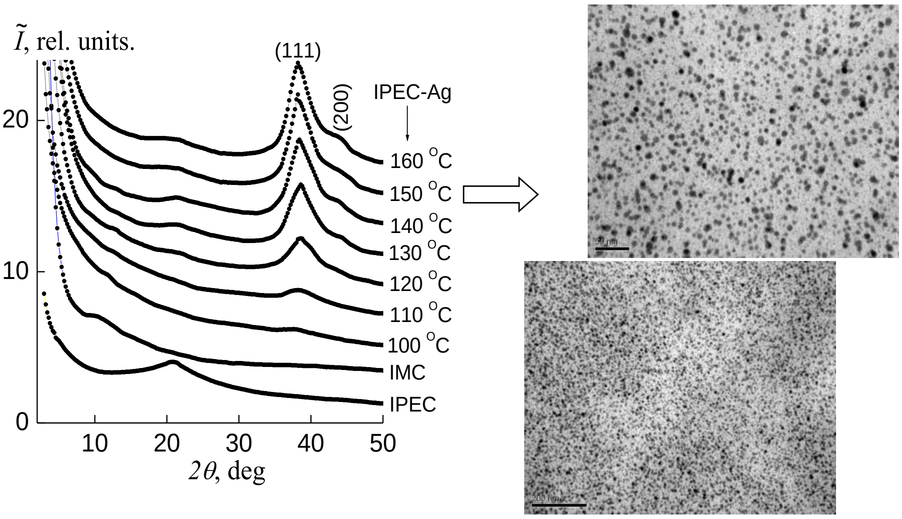

Fig. WAXS data and morphology of silver-containing nanocomposites obtained by the thermochemical reduction of Ag^+ ions in the IMC

The antimicrobial investigation of the elaborated nanocomposites revealed they possess a high antimicrobial activity against *S. aureus* and *E. coli* strains.

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A study on complexation in the system "cyclodextrin - amino acid"

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Cyclodextrins (CD) are capable to form host-guest-type inclusion complexes with many organic compounds. This property of CD is used to increase solubility, as well as hydro-, photo- and thermal stabilization of medicinal and biologically active substances. The use of CD for the preparation of nano-encapsulated drugs for medical purposes seems to be promising.

In the present work, the interaction of α-CD and β-CD with amino acids (AA) – *L*-phenylalanine (*L*-Phe) and *L*-tyrosine (*L*-Tyr) is studied. Using spectrophotometry, the formation of inclusion complexes “cyclodextrin-amino acid” in buffer solutions with pH 1.00 and 6.86 was proved, and their stability constants were determined (Table).

The geometrical and energy characteristics of the thermodynamically stable complexes of the CD···AA (Table) where an AA is present in the form of a cation (AA^+), an uncharged molecule (AA), a zwitter-ion ($AA^{+\,-}$) or anion (AA^-) were set. The enthalpy of complex formation (ΔH_{298}) was calculated taking into account the enthalpy of displacement of the water nanoclusters $(H_2O)_m$ (volume of water close to the volume of AA) from the inner cavity of the CD into solution in accordance with the process: $CD\cdots(H_2O)_m + AA \rightarrow CD\cdots(H_2O)_m + (H_2O)_m$, using the formula: $\Delta H_{298} = [H_{298}(CD\cdots AA) + H_{298}((H_2O)_m)] - [H_{298}(CD\cdots(H_2O)_m) + H_{298}(AA)]$.

The results of quantum chemical calculations (ΔH_{298}) and experimental data (K_s) indicate that the *L*-Tyr complexes with α-CD and β-CD (regardless of the pH of the medium) are stronger than those of *L*-Phe.

Table. Parameters of complex formation (enthalpy ΔH_{298} and stability constant K_s) between amino acids and cyclodextrins

Complex	AA^+ (pH 1.0)		AA (pH 4–7)		$AA^{+\,-}$ (pH 4–7)	AA^- (pH 11)
	ΔH_{298} , kJ/mol,	K_s , l/mol	ΔH_{298} , kJ/mol	K_s, l/mol	ΔH_{298} , kJ/mol	ΔH_{298} , kJ/mol
α-CD ···*L*-Phe	–25.6	13±4	–21.1	10±3	–49.2	–64.18
α-CD ···*L*-Tyr	–44.7	18±2	–45.4	12±2	–77.3	–75.5
β-CD ···*L*-Phe	–5.2	18±2	–16.2	11±2	–7.6	–27.4
β-CD ···*L*-Tyr	–41.0	103±41	–20.8	42±2	–37.0	–37.6

In the pH range 4–7, the zwitter-ions of the amino acids studied form more stable complexes in comparison with those of relative molecular forms due to electrostatic interactions.

PVA/chitosan cryogels filled by lignin: synthesis and properties

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Works in the field of polymer cryogels are a part of a wide and important branch of science - chemistry and polymer technology for technical and biomedical applications. Cryogelation is a promising method to prepare macroporous polymer gels upon freezing polymer solution with a solvent playing a role of a porogen. This leads to cryoconcentration of the polymer solution to form the macropore walls with crosslinked polymers. The textural characteristics depend mainly on the polymer-to-solvent ratio. The processes are directly related to the cooling mode, reactor design, and the ability of the polymers to form gels. Both synthetic and natural polymers can be used to form the cryogels. As a whole, there are certain problems caused by the properties of the polymers (especially solubility).

The aim of our work was to study the effects of lignin addition into poly(vinyl alcohol) (PVA)/chitosan composition on the structure and properties of the cryogels. Lignin functionalities (such as methoxy, hydroxyl, aldehyde and ketone groups, propane side chains, aromatic rings, *etc*.) can strongly affect both cryogelation-cryoconcentration and crosslinking-pore wall formation. Therefore, lignin as an additive providing certain functionalization of the cryogels can affect the morphological, textural, and structural characteristics, as well the physicochemical properties of the final materials. A question arises whether crosslinking of lignin with PVA and chitosan would take place or phase separation (stratification) occurs during the cryogelation.

Cryogelation of the PVA/chitosan/lignin system was carried out in aqueous solutions under atmospheric and high pressure conditions in cryobombs at -18°C using two concentrations of lignin (10% and 2% solution). The concentration of PVA - 2.5% aqueous solution, chitosan - 2.5% in 2% acetic acid. A 25% glutaraldehyde solution was used as a crosslinking agent.

It was established that varying the composition with chitosan, polyvinyl alcohol and lignin affects the degree of swelling of the cryogels. Thus, it is possible to vary and adjust both the textural characteristics and pore wall functionalities of the composite materials.

H_2 – TPR characterization of $ZnMoO_4$ obtained by ultrasonic method

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ZnO-MoO_3 composition is well known for applications in bolometers, scintillation detectors, humidity sensors, microwave dielectric devices, battery electrodes and catalysis. The $ZnMoO_4$ synthesized from ZnO and MoO_3 by ultrasonic method in water medium and displayed high catalytic activity in the reaction of bio-ethanol selective oxidation to acetaldehyde.

The aim of this work was studies reducing features of $ZnMoO_4$, and its comparison with mechanical mixture of initial ZnO-MoO_3. The reducing was carried out in a H_2-Ar mixture in the temperature range of 30-800°C at a heating rate of 5°C/min. The $ZnMoO_4$ and initial ZnO-MoO_3 were characterized by adsorption of N_2, XRD, ESR, SEM, TEM and FTIR methods.

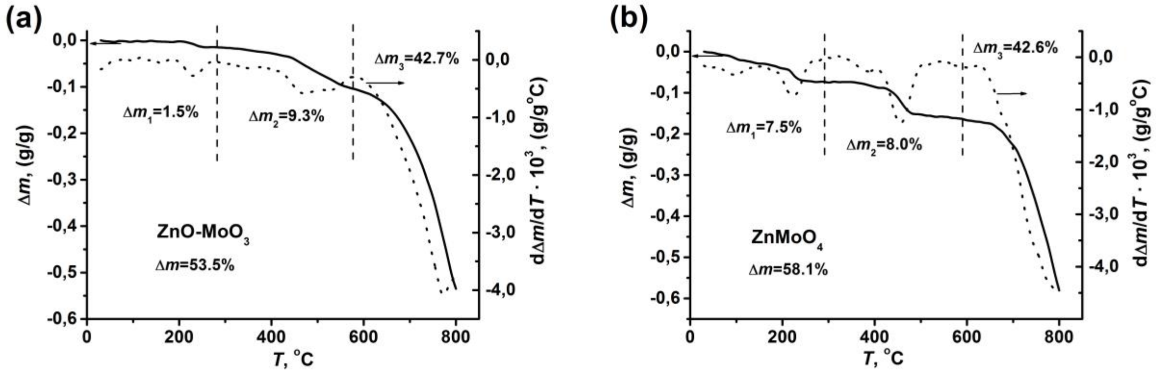

Fig. Thermogravimetric profile and relative derivative curve:
a - ZnO–MoO_3 initial, *b* - $ZnMoO_4$

TG and DTG curves (Fig.) can be conditionally split into three temperature ranges: i) at T=30-300°C; ii) 300-580°C and iii) 580-800°C. Of greatest interest is the first temperature range (30-300°C) where the mass loss in $ZnMoO_4$ is 7.5% while the mass loss in initial oxides (ZnO and MoO_3) is only 1.5%. The reducing ability of $ZnMoO_4$ could be indicating of present sites which are an active in lower temperature range. This fact could explain significant improvement of catalytic properties of $ZnMoO_4$ than the initial oxides in reaction of selective oxidation of ethanol to acetaldehyde.

Synthesis and properties of thiacalixarene based solid extractants for cerium(III) binding

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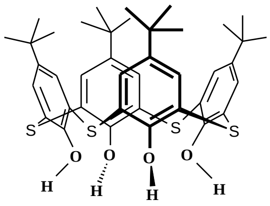
Functionalyzed calixarenes due to three dimentional cup shaped architecture are considered as promising molecular platform for design of highly effective and selective receptors of metal cations [1, 2]. In this paper we present the polymeric solid extractants (SolEx) on the base of thiacalixarene derivatives **1,2,3**.



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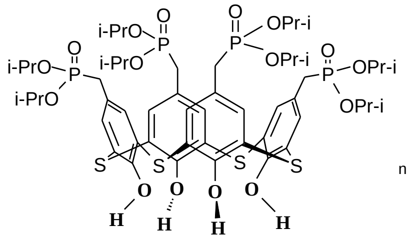

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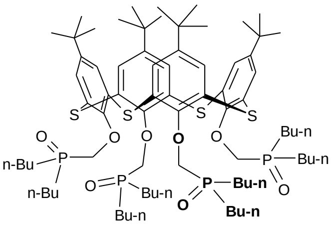

3

The SolEx were synthesized by impregnation of the porous styrene-divinylbenzene co-polymer (production of SE SMOLY) by solution of the thiacalixarenes **1-3** in *meta*-nitrobenzotrifluoride.

Sorption ability of the SolEx to Ce(III) is studied under static conditions by limited volume method in the pH range of 2-8 at the temperature of 298 K. In accordance with the kinetic studies the equilibrium occurs within 2-3 hours. The Ce(III) sorption is best described by the Freindlich model. Using the Dubinin-Radushkevich model, the free sorption energy values of Ce(III) ions on SolEx are calculated. The sorption is minimal under pH 2.3 and increases with increasing the pH value. The maximum of the Ce(III) sorption capacity (up to 80%) is observed at pH values 6 - 8 and increases in the thiacalixarenes row **1** < **2** < **3**. The efficiency the thiacalixarene SolEx exceeds those of the industrial styrene-divinylbenzene solid extractant impregnated with tributyl phosphate.

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Adsorption-structural properties of P-containing SBA-15 silicas

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The interrelation of materials on porosity, structural, morphological, and functional motives are keys for high performance in all kinds of their applications. We have investigated the changes in the adsorption-structural characteristics of ordered mesoporous silica SBA-15 after introducing acidic phosphorus-containing groups into the surface layer.

The initial mesoporous silica SBA-15-type with the definite parameters of the porous structure and high developed specific surface area was synthesized by template (Pluronic P123) method. Comparison of isotherms of nitrogen adsorption-desorption for the initial sample (SBA-15) and for silicas after chemical modification with diethylphosphatoethyltriethoxysilane (SBA-POEt) and phosphine oxide (SBA-PO) showed that there are significant changes: isotherms in the region of the hysteresis loop are shifted to the axis of relative pressures and at the same time the hysteresis loops becomes narrower (Fig.). This testifies that grafted functional groups are located not only on external surface of the silica but also on walls of the mesopores. Therefore, it is logical to expect a decrease in the total pore volume and specific surface area values after functionalization SBA-15 with P-containing groups.

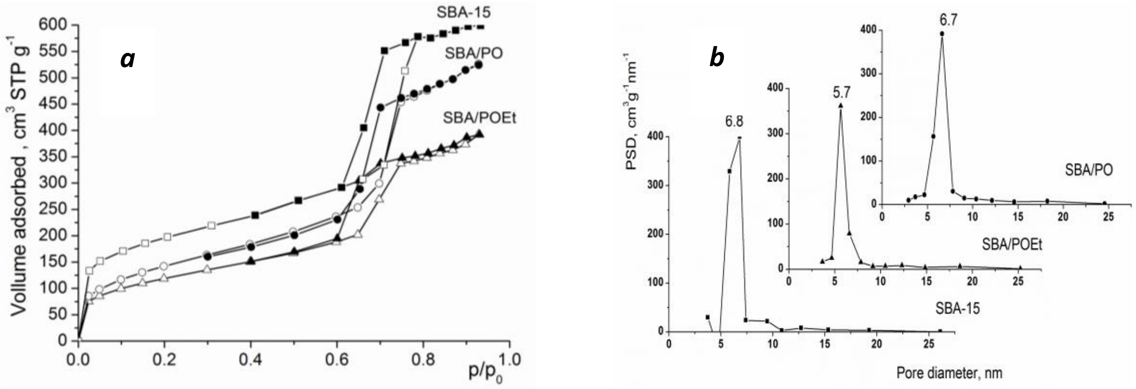

Fig. Isotherms of nitrogen adsorption-desorption (*a*) and BJH pore size distribution curves (*b*)

Nevertheless, the modified samples have a developed specific surface area and the mesoporous pore character favours the diffusion of adsorbates to active P-containing sites.

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Creation of novel organic-inorganic hybrid materials as sorbents for wastewater treatment from heavy metal ions

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Water purification is an up-to-date problem both in Ukraine and India. Currently, hardly any surface water reservoir can be attributed to the first category (with water suitable for drinking), according to the degree of water pollution, environmental and basic sanitation conditions, chemical and microbiological parameters. Mesoporous materials, primarily modified with functional groups are often considered as adsorbents of toxic substances. Their adsorption properties can be adjusted by changing: the parameters of a porous structure and the composition of the surface layer by incorporation of various groups.

Among the functional groups, phosphorus-, sulfur-, and amine-containing groups are particularly interesting. The inclusion of thiol derivatives in the structure of mesoporous organosiloxanes can provide materials with hydrophobicity and thus increase their hydrothermal stability. The simultaneous introduction of the groups of different nature in the surface layer often leads to the manifestation of the cooperative effect.

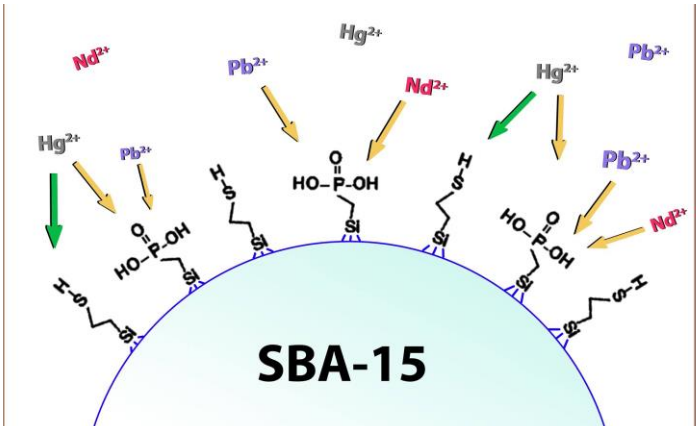

Fig. The scheme of surface layer and possible sorption reactions

Acknowledgements
Authors thank for the financial support of the present work (Bilateral project between Ministry of Education and Sciences of Ukraine and Ministry of Education of India, 2019-2021).

The influence of disperse inorganic oxides on the formation of polymer-mineral composites

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Polymer-mineral composites have unique features that combine the useful properties of both components. The formation of polymer in systems filled with dispersed minerals is significantly influence by the nature and dispersion of inorganic oxides, the type of radical initiator, and the monomer that is polymerized under these conditions.

In our work polymerization of styrene, methyl acrylate, methyl methacrylate, butyl methacrylate has been investigated in the presence of aerosil, TiO_2, PbO, V_2O_5, Fe_2O_3 and Cr_2O_3. As initiators of radical polymerization: benzoyl peroxide (BP), oligomeric peroxide of sebacic acid (OPSA), and tertiary butyl hydroperoxide (TBHP); were used.

Adsorption of peroxide initiators on aerosil, MgO, V_2O_5, Fe_2O_3, Cr_2O_3 from styrene solution was studied. The process of adsorption of the studied peroxides on the listed mineral oxides is well described by the known equation of Langmuir's monomolecular adsorption. The basic parameters of the adsorption process are determined. In the case of adsorption from solutions of compounds such as methyl methacrylate or butyl acrylate, competitive adsorption of peroxides and oxygen-containing monomers is observed. Investigation of the thermal decomposition of peroxide compounds in the presence of disperse oxides showed that the destruction of initiators runs in the solution of the monomer and on the surface of the mineral.

Peroxide adsorbed on the surface of the aerosil and Cr_2O_3 decomposes in a heterogeneous mechanism, during which no radicals can initiate polymerization. The reaction of peroxide initiators with a surface of V_2O_5, Fe_2O_3 and PbO has an oxidation-reduction nature. In the course of this interaction, free radicals are formed which can cause polymerization. The surface of disperse oxide takes an active part in the process of formation of polymer-mineral composite. In systems that contain mineral fillers, there is a breakdown of growing polymeric radicals on the surface. In the studied systems, polymerization of the investigated monomers in the solution and on the surface, or with its participation, is observed. During the formation of polymer-mineral composites, the macromolecules of the polymer are grafted to the surface. The degree of grafting of the polymer to the surface depends on the nature of the mineral and the monomer. The molecular masses of polymers that are formed in solution and in the presence of a disperse phase in the system have been found.

Highly filled composites based on polypropylene

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The highly filled composites based on polypropylene (PP) contained calcite concentrate (CC) from 5 to 50 wt.% have been prepared. The calcite concentrate is highly dispersed powder of calcite that has been treated by stearic acid and then granulated with highly-fluid PP. The content of organic component in CC is 24 wt. %. It has to be noted that 5 wt.% of elastomer, as namely polypropylene-octene block-copolymer (POBC), was added to the composite of PP and CC.

It is shown that the increase in CC content leads to the decrease of viscosity of the composites for all range of concentrations and shear strain values. This result is contradicted to the traditional rules for melt flows filled with hard additions where the viscosity increase takes place. It is established that value of melt index is increased for the samples contained up to 50 wt.% of CC content: from 3.1 g/10 min for pure PP to 6.6 g/10 min for composite contained 50 wt.% of CC. It is shown that the presence of CC affects the melting and crystallization processes of PP. At low (5 wt.%) and medium (10 - 20 wt.%) contents, T_m and T_c temperatures are increased from 168 to 169-170 °C and from 115 to 117-118 °C, respectively. The melting intervals are narrowed from 42 °C for PP to 38-34 °C for composites with 30 - 50 wt.% CC contents while the crystallization temperature is noted from 18 to 16-15°C for composites with high CC contents. The increase in phase transition temperatures points on the formation of bigger and perfect crystallites whereas the narrowing of temperature intervals of phase transitions indicates on the formation of crystallites with more uniform sizes. The influence of CC on rheological behavior and temperature characteristics of phase transitions is connected with plastifying effect of modifier chains on calcite surface and the presence of highly-fluid PP as the polymer-basis. The presence of CC and CC together with POBC leads to the decrease in effective activation energy of oxidative thermodestruction that can be explained by the decrease of binding in system due to the presence of modifying agents.

Adsorption of toxic organic substances on biochar and composites containing carbon nanomaterials

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The subject of this work is to develop multifunctional adsorbents for water decontamination: the materials give the possibility to remove both inorganic ions and organic pesticides from diluted aqueous solutions. The samples of biochar have been synthesized by chemical carbonization of disaccharide (lactose) and polysaccharide (dextrin). Other type of adsorbents is the composite included hydrated zirconium dioxide and multiwalled carbon nanotubes (≈2 mass %). The composites were synthesized by deposition from sol of insoluble zirconium hydroxocomplexes, in which the nanosized GO particles were dispersed. The adsorbent as well as its constituents were investigated with XRD and XPS analysis, FTIR spectroscopy, TEM and SEM. BET measurements were also applied. It has been found that the nanotubes cover the particles of inorganic oxide. On the other hand, the composite involves agglomerated nanotubes. Several groups, which are characteristic for GO, were found: vibration spectroscopy indicated C–OH (attributed both to hydroxyl and carboxyl groups), C=O (related to carboxyl groups) and C–O–C bonds (epoxy groups). Among them, carboxyl and phenol groups are responsible for ion exchange. At the same time, hydrophobic regions of the nanotubes provide adsorption of organics. Main regularities of adsorption of toxic species (Pb^{2+} cations and $HCrO_4^-$ anions) were studied. Adsorption of such pesticides as epoxiconazole, quizalofop-ethyl, tebuconazole, acetamiprid, carboxyn, thiamethoxam from the mixed solutions was also researched. For instance, the solution contained initially 0.85-170 mg dm^{-3} of carboxyn and 0.35-70 mg dm^{-3} of epoxiconazole. Depending on initial content of pesticides in a solution, adsorption capacity of the composites reaches, for example, up to 79 mg g^{-1} (towards carboxyn) and up to 7 mg g^{-1} (epoxiconazole). When the most diluted solution is used, the pesticide content in water is lower than maximal allowable concentration.

Regarding biochar, the degree of removal of toxic organic compounds from water is above 99%. In the case of epoxyconazole and carboxin, adsorption capacity was estimated as 79 and 120 mg g^{-1}, respectively.

Sorption of ^{110}Ag by MnO(OH) particles from aqueous solutions

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At present, the significant amounts of solutions with low silver content are accumulated, especially in industrial and waste water of watch and jewelry manufactures; used solutions from photo and film production; sewage of electronic and electrotechnical industries. To extract silver from such solutions, expensive and non-regenerable ion exchange resins are mainly used, that is not economically profitable. As an alternative to ion exchange resins, an promising inexpensive sorption material — the manganese oxohydroxide MnO(OH) could be used.

In the present work, the nano-sized particles of MnO(OH) are synthesized; the sorption properties of this material towards ^{110}Ag radionuclide at different values of pH of the solution are studied; the equilibrium and kinetic patterns of sorption of Ag^+ ions from model aqueous solutions with MnO(OH) are investigated.

MnO(OH) ability to sorb ^{110}Ag radionuclide was studied under static conditions by the method of limited volume at 293 K and pH value from 2 to 8. The efficiency of sorption extraction of silver ions was determined by values of the ion distribution coefficients (K_d, dm^3/g) and sorption coefficients (K_s, %).

To determine the order of the reaction, the data of the kinetic experiments were processed using the pseudo-first and pseudo-second order kinetic models. The model of pseudo-second order kinetics describes the experimental data the most adequately. This testifies to the limiting stage of the sorption process is chemisorption, the effect of diffusion stage is insignificant. Sorption isotherms of silver ions on manganese oxohydroxide MnO(OH) were processed using the Langmuir, Freindlich, Redlich-Peterson and Langmuir-Freindlich models of sorption isotherms. It is shown that the sorption of silver ions is best described by the Freindlich model. Using the Dubinin-Radushkevich model, the values of free sorption energy of silver ions are calculated. By its nature, oxohydroxide is weakly acidic ion exchanger, containing hydroxo-groups, thus the silver sorption is minimal at pH 2 and sharply increases with increasing the pH value.

Analysis of the sorption characteristics obtained by the sorbent studied allows MnO(OH) to be recommended for the concentration and separation of silver ions from technological waters.

Investigation of the influence of aluminium content on spectral properties of Eu(III) chelates doped in mixed SiO_2-Al_2O_3 matrix

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Lanthanide(III) complexes are characterized by narrow band luminescence in a wide spectral range due to transitions between 4*f*–sublevels and large values of excited state lifetimes. However, lanthanide systems are characterized by a high probability of nonradiative energy losses, which lead to a decrease in the efficiency of 4*f*-luminescence. Therefore, the development of approaches to minimize them is one of the urgent tasks. The introduction of coordination compounds into organic-inorganic hybrid materials allows, on the one hand, to minimize the processes of emission quenching, and on the other hand, to achieve high values of emission intensity of materials due to the high concentration of radiating centers. Hybrid materials can be obtained in the form of gels, glass, films, fibers, ceramic powders and nanoparticles using different types of sol-gel method.

Inorganic matrices, primarily silicon dioxide obtained by sol-gel method, are widely used as carriers in the production of hybrid materials. The attention of researchers is also attracted by hybrid materials based on aluminium, titanium, zirconium oxides, *etc*. A few attempts to increase the luminescent characteristics of materials through the use of mixed matrices are known. However, such data do not allow to establish how the transition from silica to oxides of other elements affects the luminescent characteristics of lanthanide complexes.

The present work discusses the results of spectroscopic studies of hybrid materials based on adducts of Eu(III) tris-*β*-diketonates and 1,10-phenanthroline that were introduced into the mixed inorganic matrices with different ratio of SiO_2/Al_2O_3. Introduction of Eu(III) complexes was done using both covalent and non-covalent interaction. The features of synthesis of such materials and properties of lanthanide-centered luminescence in the visible region, as well as the prospects for practical use of resulting materials are discussed.

Influence of synthesis conditions on the physical and chemical properties of the yttrium iron garnet

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Ferrites with the spinel structure found a wide use in many fields of human activity due to their characteristics such as the high electric resistivity, low magnetic losses beyond the ferromagnetic resonance (FMR) area, wide range of saturation magnetization and extremely thin FMR curve, for example in magneto-optical data recording devices, non-reciprocal microwave devices for communications such as circulators, isolators, filters, phase shifters, *etc*. At the same time, modern communications development requires the preparation of new materials with the high physical and chemical characteristics.

The main problem of yttrium iron garnets is synthesis of weakly agglomerated, small-dispersive (nanoscaled), single phase particles. Such particles will allow increasing of physical and chemical properties of named materials by obtaining the high density ceramics, moreover it will allow answering on a number of questions about a connection between structure features and properties, others. Conventionally the solid-state synthesis is used for the synthesis of ferrites with the garnet structure, but this method doesn't provide the chemical homogeneity of product and requires high temperature of synthesis (1200°C), also using of solid state synthesis leads to a pollution of powders during the long-lasting milling process.

This study offers the synthesis of yttrium ferrites doped by aluminum, manganese and chrome by methods of co-precipitation and sequential precipitation of hydroxides from aqueous solutions. Aqueous solutions of metal nitrates $Y(NO_3)_3$, $Fe(NO_3)_3$, $Mn(NO_3)_2$, $Al(NO_3)_3$, $Cr(NO_3)_3$ were used as the starting reagents. Aqueous solutions of alkali (NaOH) and ammonia were used as the precipitators.

It was shown that the synthesis method and precipitator (NaOH or NH_4OH) make a significant impact on the particle's agglomeration. It was established that obtained precipitates are amorphous and requires an additional heat treatment, but particles stay nanoscaled with the sizes 50-90 nm even after the heat treatment at 900°C depending on a synthesis method. It was shown, that using sequential precipitation of hydroxides the filtering coefficient increases for three times, that allows significantly reduce a time of precipitates filtering and washing from natrium ions. Using synthesized nanoparticles dense ceramics was obtained. An influence of synthesis methods on electrophysical properties of ferrites with the garnet structure was shown.

Effects of photoactivation of amino acid tryptophan on silver nanoparticles formation

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Silver nanoparticles (Ag NPs) are well known for their antibacterial properties that can be used for medical purposes. Ag NPs on their own or as a component of complex nanoobjects can find an application in diagnostic and treatment of tumors. In turn, the anti-cancer effect of Ag NPs can be varied and improved by changing the size of nanoparticles.

Ag NPs is possible to obtain in the presence of tryptophan (Trp), an essential amino acid for the human body, used as a metal reducing agent to decrease the toxicity and enhance the efficiency of nanoparticles in biological systems. As chemical redox reaction between Ag^+ and Trp involves photoactive indole ring of amino acid, the additional photoactivation of the system with UV irradiation can affect the process of particle formation and, as a result, morphology of Ag NPs. In the work the influence of UV-C LED irradiation of Ag^+/Trp system at 278 nm on properties of Ag NPs was investigated. The experimental parameters of the irradiation (0.4, 0.6 and 1.0 mW/cm^2) and temperature of reaction (25, 40 and 60°C) were changed in order to study the kinetics of photochemical process, size and size distribution of the prepared silver NPs. Photochemical formation of Ag NPs can be accelerated up to 10 times with an increase of the temperature from 25 to 60°C. At the same time, the average size of nanoparticles can be decreased from 50 to 20 nm, accompanied with the shift of the position of silver plasmon resonance band maximum from 422 to 412 nm. Thus, optimal UV irradiation parameters and temperature of reaction can be applied to obtain Ag NPs with tailored properties.

Adsorption of proteins on nano-silica modified with antimicrobial drugs

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The research is devoted to the preparation of new nanocomposites on the basis of silica matrices with antiseptic properties and to the investigation of their sorption capacity for proteins in the presence of antimicrobial drugs. Nanocomposites were prepared by impregnation of ornidazole and urotropine on the surface of silica. Nanosilica (A-300) was used as a matrix. Ornidazole (1-(3-chloro-2-hydroxypropyl)-2-methyl-5-nitroimidazole) and urotropine (hexamethyleneteramine) were used as substances-modifiers.

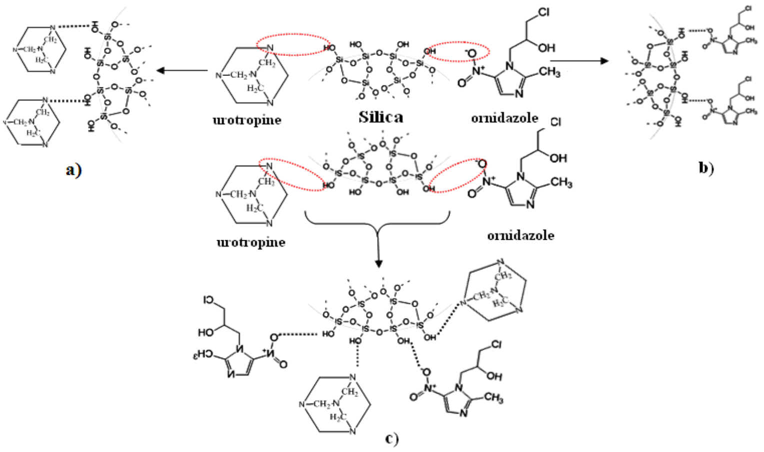

Fig. Scheme for the preparation of nanocomposites: *a*) silica + urotropine (urosil); *b*) silica + ornidazole (ornidasil); *c*) combined nanocomposite made from silica + urotropine and ornidazole (ornurosil)

Adsorption of proteins on the surface of the received nanocomposites was investigated under static conditions and compared with adsorption on unmodified silica. The results of the study of the sorption capacity of nanocomposites relatively to the proteins showed that the maximal amount that ornidasil was able to adsorb was 162 mg/g, for urosil it was 207 mg/g, for the combined composite ornurosil it was 209 mg/g, during the exposure time of 48 hours with the temperature of 18 °C and pH = 4.6 (Table).

Table. Sorption capacity of the nanocomposites relatively to a protein depending on the duration of exposure

	Sorbent			
	Initial silica	**Ornidasil**	**Urosil**	**Ornurosil**
Exposure time	**The amount of protein adsorbed from the BCA model solution, mg/g of sorbent**			
6 hours	146	132	160	135
12 hours	153	148	189	167
24 hours	178	160	200	181
48 hours	189	162	207	209

The obtained results indicate that the prepared nanocomposites possess a sufficient proteonectic ability, which opens up new possibilities for the creation of combined medications on the basis of silica and biologically active substances.

Characterization of the lithium iron(II) phosphate/carbon nanocomposite by Raman and XPS spectroscopy methods

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Lithium iron(II) phosphate is a promising cathode material for lithium ion batteries. One of the main drawbacks of $LiFePO_4$ is the low electronic conductivity. The classical conductive agent introduced to modify electrode materials is carbon, which possesses high conductivity [1].

The Raman spectra of the $LiFePO_4$/C composites obtained from an annealed powder with glucose and malic acid have pronounced D (~ 1340 cm^{-1}) and G (~ 1600 cm^{-1}) peaks, as well as two additional bands at ~ 1200 and ~ 1520 cm^{-1} obtained after the deconvolution of main peaks. The ratio of peak intensities of lines D and G (I_D/I_G) has a value of 1.02-1.06 for the material obtained after glucose carbonation and 1.01-1.02 for $LiFePO_4$/C annealed with malic acid, which means that there is predominantly sp^2 carbon which is characterized by high electron conductivity.

We used X-ray photoelectron spectroscopy (XPS) to determine the concentration of iron(II) and iron(III) on the surface of $LiFePO_4$ crystals and the nature of the carbon coating on it. The C analysis of 1*s*-peak was performed with its expansion into components. The spectrum consisted of several components of different nature, where the most intense peak (77.5%) with an energy of ~ 285 eV characterizes the presence of sp^2 carbon with bonds C-C or C=C. Also, there are peaks that can be classified as oxygen-containing functional groups.

The XPS Fe2$p_{3/2}$ spectrum of non-annealed $LiFePO_4$ after synthesis and annealed $LiFePO_4$/C composite was obtained. For both samples, the total content of iron(II) is ~ 65%. These results confirm that the organic precursor carbonization regimen on $LiFePO_4$ surface proposed by ourselves (700 °C, 1 h) does not lead to the oxidation of the material.

Using the XPS method, the thickness of the carbon coating on the $LiFePO_4$/C surface was estimated. The lower iron response in the analysis of annealed material is indirectly confirmed by the presence of a carbon coating of optimum thickness (up to 4 nm) obtained by thermal decomposition of the organic precursor.

1. Z. Yang, Y. Dai, S. Wang, J. Yub, J. Mater. Chem. A. **4** (2016) 18210

Elemental-phase composition study of por-Si/c-Si heterostructure's interfaces obtained by electrochemical etching

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Surface area in por-Si/c-Si heterostructures sufficiently grows up compared to c-Si samples. The degree of porosity and thickness of porous layer affects its value up to 2-3 orders of magnitude. So, this developed surface is obviously related with high concentration of adsorption centres, what influences various applications of porous Si, i.e., photo luminescent, biomedical *etc*.

Por-Si/c-Si heterostructures were obtained by electrochemical etching of 400 μm thick *n*- and *p*-type c-Si (111) substrates in 25% HF ethanolic solution. The porosity varied within 20-80% range with a 20-30 μm thickness of porous layer. Thus obtained por-Si/c-Si heterostructures were rinsed in water and dried. The Auger spectra were acquired in the $dN(E)/dE$ derivative mode by cylindrical mirror analyser using 3 keV primary electron beam energy. The secondary ion mass spectrometry (SIMS) data were obtained in the ultrahigh vacuum chamber on LAS-600 RIBER unit with 1 keV energy and ion current density of $j=10^{13}$ ion/cm$^2\cdot$s of Ar$^+$ sputtering ions, resulting in low rates surface sputtering about 2-3 Å/min.

The Auger electron spectroscopy studies give evidence that for c-Si surfaces, even for those obtained in the high and ultrahigh vacuum, the formation of carbon-oxygen adsobate coatings is characteristic. The phases of atomically clean or hydrogenated (SiH_x) silicon and also silicon- oxygen-carbon amorphous $Si_yO_xC_{1-x-y}$ thin film coatings are present on real por-Si surfaces. Besides, some surface areas contain a residual background of chlorine, fluorine and nitrogen.

Just as in the case of AES spectra, in the SIMS ones of the por-Si interface in por-Si/c-Si heterostructures acquired immediately after the etching, washing and drying processes, there are present the elements and compounds indicating that the samples are oxidized and contaminated with hydrocarbons. This is evidenced by the peaks of O^-, OH^-, $SiOH^-$ and SiO_2^- ions along with the peaks of C^-, C_2^-, CH^-, $C_2H_2^-$.

After the ion etching of approximately 15 Å surface layer thickness, the intensity of all above peaks is reduced by almost twice, except for the halogen (F^-, Cl^-) ones.

New insight into the physical origin of phase angle in Warburg finite length diffusion impedance

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The basis of theoretical studies on the electrode impedance consists in revealing the nature of processes occurring on electrode/electrolyte interface. In 1899, Warburg obtained the impedance of a semi-infinite transport layer attached to a planar electrode. Warburg's result has been extended to the transport layer of a finite thickness. In this work, we develop a simple physical model, which describes the origin of phase angle of the Warburg finite length diffusion impedance. We show that diffusion results in a phase delay of the surface concentration of species with respect to current. The phase angle of the Warburg finite length diffusion impedance has a maximum that does not depend on either the Nernst diffusion layer thickness values or the diffusion coefficient of species. The effects of the Nernst diffusion layer thickness, charge-transfer resistance, diffusion coefficient, double layer capacitance, and electrolyte resistance on the behavior of phase angle are discussed.

Fig. shows the complex-plane plots of the interface impedance for different R_{ct} values. The diagram consists of two loops. The left loop corresponds to the charge-transfer impedance. The size of the loop depends on the R_{ct} value. The radius of the semi-circle is equal to $R_{ct}/2$. The size of the right loop does not depend on the R_{ct} value.

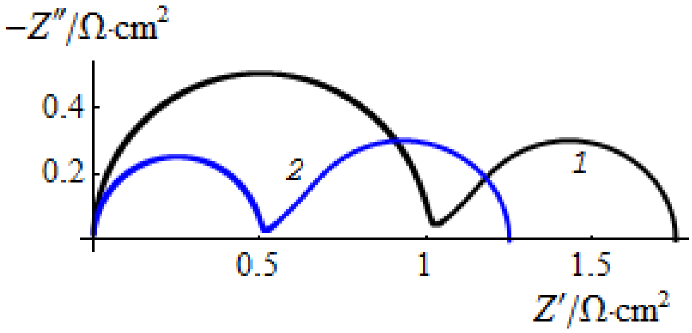

Fig. Niquist plots of the interface impedance for different values of charge - transfer resistance $R_{ct}/\Omega\cdot\text{cm}^2$ as follows: (*1*) 1; (*2*) 0.5

The effect of the presence of organic and mineral components in AM1-based composite systems on morphological characteristics of tomato sprouts

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Hydrophobic silica AM-1 easily forms composite systems, since they have a high degree of adhesion to the seeds surface in a wide range of concentrations using trace elements, plant growth regulators, as well as mineral and organic fertilizers and nanofungicides.

The aim of our work was to compare the morphological characteristics of tomato sprouts, the seeds of which were processed with composites based on hydrophobic silica AM-1 with the content of a mineral or organic component.

For the research, “Cherry” tomato seeds of red and yellow colors were selected, which were processed with two types of composite materials: hydrophobic silica with a mineral component (AM-1/min) and hydrophobic silica with an organic component (AM-1/org), and the original AM-1.

Leaves of both yellow and red tomatoes processed with AM-1/min and pure AM-1, have got fewer it number compared to control (Table 1), small sizes and dark green on the outside and purple color from the bottom were observed. Stems are thin and vertical with the purple color of the lower part of it. The presence of purple in sprouts can be a sign of phosphorus deficiency in the soil. Seeds, processed using the composite AM-1/org and control, are characterized by a pale green leaf color, large diameter of the leaf blade and their number (5-6 pieces).

Table. Morphological characteristics of tomato sprouts

Samples	Roots red/yellow, cm	Stems red/yellow, cm	Number of leafs red/yellow	Diametr of leafs red/yellow	General look
Control	4.5/2.5	6.5/6.7	5/5	2.8/3.6	lie down
AM-1/org	5.5/4.3	6.4/6.9	5/6	3.5/3.7	lie down
AM-1/min	2.8/4	5.8/5.0	4/4	2.6/2.7	thin stems
AM-1	3/5	5.2/5	4/4	2/3	thin stems

Thus, the optimal composition of the nanocomposite system for pretreatment of seeds, based on hydrophobic silica, should combine both mineral and organic components in its.

Bile acid adsorption on the chitosan-containing silica surface

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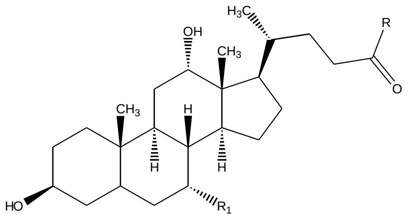
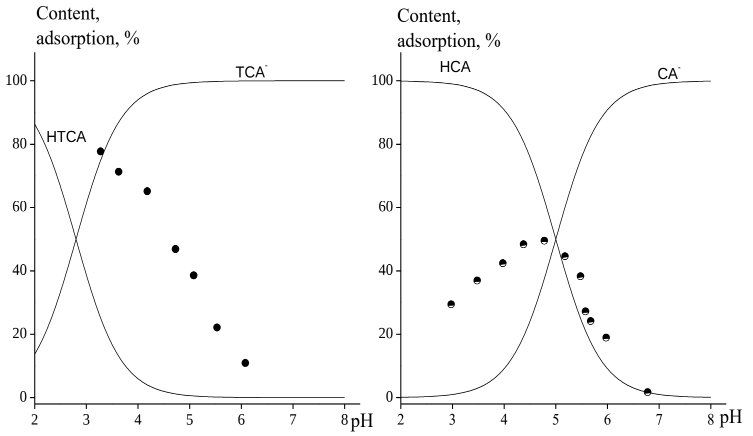
Bile acids (BA), natural surfactants, are involved in the process of digestion and assimilation of fatty foods. Since bile acids are products of the decay of cholesterol in living organisms, their adsorption on the surface of sorbents can be considered as a possible way of removing BA from enterohepatic circulation and additional cholesterol splitting. Attempts were made to find efficient sorbents with high ability for binding bile salts, to improve selectivity and biocompatibility. The combination of chitosan, which is a natural polymer containing amino groups, with silica appeared to be promising for the extraction of bile salts from aqueous solutions and, possibly, biological fluids. For this aim the adsorption of two bile acids, cholic and taurocholic, from aqueous solutions onto the surface of chitosan-silica composite was studied.



cholic acid, $R=R_1=OH$;
taurocholic acid,
$R=NHCH_2CH_2SO_3H$,
$R_1= OH$.



Solution speciation and adsorption of taurocholic (HTCA) and cholic (HCA) acids:
C_{sorbent} = 5 g/l, C_{BA} = 0.1 mmol/l

The adsorption of bile acids is due to the electrostatic interaction of their anionic forms with protonated amino groups of chitosan. The deprotonation constant of NH_3^+-groups, pK_a is 6.5, that means that at pH = pK_a only half of the groups remain protonated. The decrease in the adsorption of BA with increasing pH can be explained by a diminishing of part of protonated amino groups, although in the solution, the anions of BA prevail.

Thus, the principal possibility of using chitosan-containing silica as a sorbent for binding bile salts is shown. The combination of inorganic (silica) and organic (chitosan) components in the composite could lead to an improvement in its physicochemical properties and make it more pleasant for using in medical practice as bile acid sequestrant.

Modification of the surface of montmorillonite nanoparticles with a polar modifier containing available amino groups

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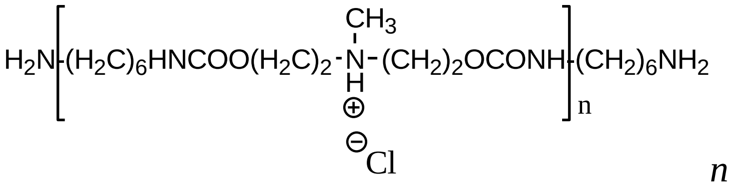
One of the most interesting and promising directions in the polymer and material science in recent years is the development of principles for producing polymer nanocomposites. One of the most important ways to create nanoparticles for introduction into the polymer matrix is the modification of the surface of inorganic nanoparticles with organic compounds.

Natural inorganic structures such as montmorillonite (MMT) are commonly used to produce polymer nanocomposites. Surface modification of MMT nanoparticles with chemical adsorption of organic cations has opened the opportunities for compatibility of silicate nanoparticles with polymer.

In order to create a nanofiller for polar MMT-based heterochain polymers, a MMT surface' modifier was synthesized that contains polar (urethane) fragments and available reactive amino groups.

The new oligourethanamine amonium chloride modifier (OUAAC) is a cationic surfactant, which contains reactive amino groups that are located at the ends of the molecule and are available for reactions with the functional groups of the corresponding monomers.

General chemical scheme of cation oligourethanamine amonium:



$$H_2N\left[(H_2C)_6HNCOO(H_2C)_2-\overset{CH_3}{\underset{\underset{\ominus Cl}{\overset{H}{\oplus}}}{N}}-(CH_2)_2OCONH\right]_n(CH_2)_6NH_2$$

$n = 1 – 3$;

Intercalation of modifier into the interlayer space of MMT was confirmed by X-ray analysis. The content of organic component in the MMT modified with OUAAC was determined by thermogravimetric analysis.

The determination of the number of amino groups in OUAAC was carried out by the method of acid-base titration. OUAAC IR spectra demonstrate the presence of ionic and amino groups.

The new modifier – OUAAC provides high affinity of MMT/OUAAC with polymer matrix due to the possibility of physical and chemical bonds formation. New method of MMT modification is universal and can be applied to MMT of various origins (deposits).

Experimental investigation of interface interaction in graphene-epoxy nanocomposites

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Thermal stability and dielectric properties of epoxy nanocomposites filled with multi-layered graphene nanoplatelets (MLGNP) have been studied by using a programmable thermal desorption technique combined with a mass-spectroscopic detection equipped with the single-pole mass-analyzer MX7304A and infrared spectroscopy equipped with the Thermo Nicolet NEXUS FT-IR spectrophotometer in the range of 400-4000 cm^{-1} of the resolution of 2 cm^{-1}.

MLGNP have been prepared by using an ultrasonically-assisted electrochemical technique. The scanning electron microscopy showed the particles consisting of several dozen loosely bound graphene layers with an area of at least 5 × 5 μm. The specific surface area of graphene was found to be about 790 m^2/g from adsorption–desorption isotherms according to the standard BET method by using “Autosorb Station 3” apparatus. ED-20 epoxy was the polymer matrix for the nanocomposites and MLGNP-loading (C_f) varied as 1.0, 2.0 and 5.0% by weight. The nanocomposites were prepared by pouring a suspension with graphene particles into the liquid resin.

Mass-desorption spectra have been decoded for a number of m/z-volatile moieties (here m is the moiety mass and z is its electric charge). The amount (Q_i) of the i-th moiety was determined from expression

$$Q_i = A \int_{T_1}^{T_2} I_i(T)\,dT,$$

where A is a dimension parameter, $I_i(T)$ is the temperature dependence of the thermal desorption intensity of the i-th moiety, T_1 and T_2 are the temperature limits for integration. The parameter $1/Q_i$ can be serve as a quantitative measure for thermal resistivity of the nanocomposites.

It has been found that the loading $Q_i(C_f)$ dependences for various m/z-moieties are nonmonotonic descending reaching their minimal values at C_f=1%. It’s remarkable that $1/Q_i(C_f)$ correlate well with the loading dependences of the intensities for the absorption bands in the nanocomposite’s IR-spectra. The effect can be treated as a result of the polymer structure transformations upon interaction of macromolecule atoms with the active surface sites of MLGNP.

Photocatalytic aerobic aromatization of substituted 1.4-dihydropyridines in the presence of crystalline carbon nitride

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Within the scope of work we have synthesized crystalline carbon nitride (CCN) by thermal treatment of bulk g-C_3N_4 in the molten salts of KCl and LiCl [1]. It has been shown that the material has a layered structure and mainly consists of plates 20–30 nm wide and about 200 nm long (Fig.). The activity of the nanostructured material was investigated in the reaction of photocatalytic aerobic aromatization of 1,4-dihydropyridines under visible light (($\lambda > 400$ nm). It was established that initial 1,4-dihydropyridines can be easily aromatized to the corresponding aromatic product with a high conversion and selectivity level. The presence of the nanostructured photocatalyst increased rate of the investigated process twice compared to solely photolysis.

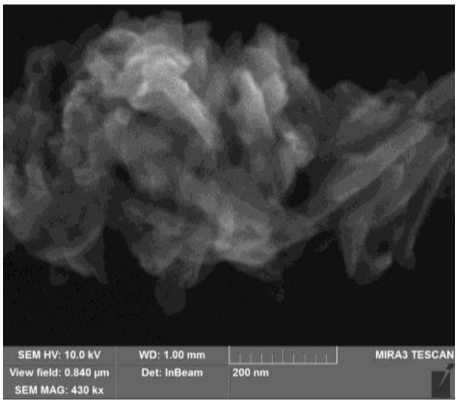

Fig. SEM images of CCN

The high photoactivity of the nanostructured CCN can be attributed to the intense absorption of visible light, the small particle size and developed surface.

1. N.S. Andryushina, V.V. Shvalagin, G.V. Korzhak, G.Ya. Grodzyuk, S.Ya. Kuchmiy, M.M. Skoryk, Appl. Surf. Sci. **475** (2019) 348.

Accommodation of the reaction energy by the electron channel on the surface of planar heterostructures

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The processes of energy dissipation on the surface via elementary processes, including electron and phonon excitations, at the moment of time when the act of formation of an excited product in an exothermic catalytic reaction just occurs, is an integral part of surface physics and chemistry. The exothermic chemical reaction, as well as the interaction of photons with the surface, leads to electronic excitation of the crystal, i.e. to the generation of hot electrons in metals and non-equilibrium carriers in semiconductors. This phenomenon can be used to create chemical current generators (CCG) for the production of autonomous power supplies along with fuel cells (FC).

FC consists of 2 electrodes on which chemical reactions occur, separated by an electrolyte. The benefits of FC are a high efficiency, environmental friendliness, and autonomy. The disadvantages of FC are high cost of FCs and electricity, limited service life, slow start-up, inertia, *etc*. Virtually all the disadvantages of FCs are caused by electrolyte.

In the 1990s, a new phenomenon was discovered: the generation of non-equilibrium current carriers in metals under the action of a chemical reaction. This leads to the generation of current in Schottky diodes. In contrast to FC, these devices lack an electrolyte and they should not have the disadvantages associated with it. The phenomenon of non-equilibrium chemogeneration of current is quite young. Therefore, CCG have low efficiency at the moment. This is due to the fact that the chemo-current mechanism was not developed.

We have developed a chemo-current mechanism and obtained dependences of the chemo-current output and the efficiency of such CCG. The characteristics that affect the yield and efficiency of the considered CCGs are revealed. The theoretical value of the maximum efficiency of CCG on the Schottky diode (36.8%) and planar heterostructures (up to 50%), which is comparable with the efficiency of internal combustion engines, has been determined. And although CCGs have a much lower efficiency, compared with FCs, due to the absence of electrolyte, they will have minimal mass and size, higher values of specific power, will not have inertia (because in CCG, the generation of non-equilibrium carriers occurs in the act of chemical interaction during a time of the order of 10^{-12} s), which is important, for example, for cars. Thus, the disadvantages associated with the electrolyte disappear in CCG and they can be used for automobiles, portable and stand-alone power supplies, *etc*.

Hydrogen peroxide decomposition by kaolin clay modified with nanoceria

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Nanoceria attracted attention due to it's unique redox properties, which are determined by surface defects - the presence of cerium atoms in two degrees of oxidation. For the nanoscale particles it's surface, and hence the number of defects (Ce^{3+} / Ce^{4+} ratio), increases. The aim of this work is synthesis of a number of new nanocomposites kaolin / cerium oxide with decorator different content, identification their physical and chemical properties, experimental determination of both: the synthesized materials catalytic activity and activation energy (E_a) for the model reaction of hydrogen peroxide (HP) decomposition.

A series of nanocomposites kaolin / cerium oxide were synthesized by reaction of cerium nitrate deposition in an aqueous medium without stabilizers at room temperature: $4Ce(NO_3)_3 + 12NaOH + O_2 = 4CeO_2 + 12NaNO_3 + 6H_2O$.

Atomic emission spectrometry, TEM, SEM, IR- and UV diffuse reflection spectroscopy, electron- and X–ray diffraction methods were used for properties characterization of the kaolin nanomaterials with CeO_2 different content.

Catalytic activity of investigated materials was estimated by monitoring the reaction of hydrogen peroxide decomposition. Volumetric method was used to determine the kinetic of HP decomposition. Maximal reaction rate was calculated from kinetic curves for different HP concentration (1–11 %). The catalytic activity of the synthesized nanocomposites, pristine kaolin and pure nanoceria was investigated in a model reaction of H_2O_2 decomposition in pH range 8.5 – 10.5 and compared with the enzyme catalase activity. To determine the activation energy of the reaction, the reactions of HP decomposition were done at five different temperatures: 20, 25, 30, 35, 40 °C (pH 10.0). The graph of logarithm of reaction constant dependence $1/T$ (K) allows to calculate E_a.

It was shown that the catalytic activity of nanocomposites kaolin / cerium oxide correlates with modifier content. The dependence of the synthesized nanocomposites activity on pH is extreme with maximum at pH 9.5-10.0. Catalase mimetic activity of studied materials in terms of 100 % content of cerium oxide and activation energy of the hydrogen peroxide decomposition reaction by them correlate with nanooxide particle dispersion and ceria surface defects, evaluated as $I_{UVSCe}{}^{4+}/I_{UVSCe}{}^{3+}$ ratio. Increasing the amount of modifier, the size of nanocrystallites and defect of their surface reduces the activation energy.

Theoretical analysis of adsorption of various compounds onto hydrophilic and hydrophobic silicas

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Experimental investigations (using FTIR, Raman, NMR, XPS, DSC and other methods) of adsorption phenomena give average and sometimes too general pictures with no some important detailed information. This information could be obtained using theoretical modelling of the adsorption phenomena using appropriate methods and models. More accurate information could be obtained using *ab initio* (with MP) and DFT with large basis sets with consideration of the effects of temperature (with various dynamic approaches), media (with solvation models), lateral interactions of adsorbates, sizes of solid particle models (cluster approach) or expanded cells (periodic boundary conditions), *etc*. However, the most accurate methods/models of the adsorption phenomena need great computational resources (*e.g*., supercomputers). Some restrictions in the latter lead to a problem of a choice of appropriate models and methods/basis sets. Represented results were obtained using two Xeon (two Platinum 8160 chips with 96 threads and two Xeon E5-2696-V3 chips with 72 threads) based workstations. In the models (Fig.), 30-50 polar (H_2O, NH_3, CO_2) and nonpolar (C_6H_6, N_2, CH_4 or fragments of polydimethylsiloxane, PDMS) molecules and some their mixtures were adsorbed onto hydrophilic silica (22-44 tetrahedra) and hydrophobic silica clusters with dimethylsilyl or trimethylsilyl groups. Quantum chemical calculations were carried out using a density functional theory (DFT) method with a hybrid functional ωB97X-D with the cc-pVDZ or aug-cc-pVTZ basis sets using the Gaussian 09 (D.01) and GAMESS 18.R3 program suits. The solvation effects were analyzed using the SMD method. The gauge-independent atomic orbital (GIAO) method was used to calculate the NMR spectra of certain systems (up to 400 atoms). Larger structures (up to 18000 atoms) were calculated using semiempirical PM7 method (MOPAC 2016).

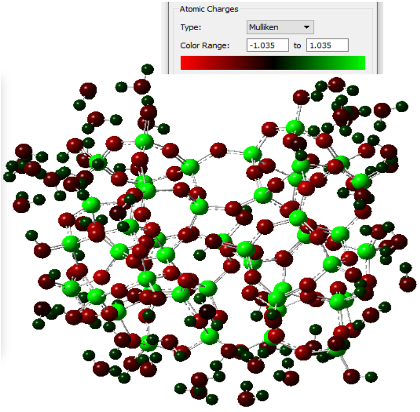

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Fig. A silica cluster with 44 tetrahedra and bound $40H_2O$ (ωB97X–D/cc–pVDZ)

Investigation of fumed silica surface accessibility with BSA interaction by adsorption and IR spectroscopy methods

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The aggregation processes in silica dispersions can potentially affect its sorption properties, especially in relation to proteins macromolecules. The accessibility of the surface of non-porous high disperse silica A-300 (S_{BET}=318 m^2/g) during the adsorption of bovine serum albumin (BSA, M=68000) has been studied in the work. The BSA adsorption isotherms are well described by the Langmuir equation; the time for establishing the adsorption equilibrium does not exceed 1 hour. It was shown the BSA monolayer capacity (500±30 mg/g) is 2.5 times the maximum adsorption value for linear macromolecules, which fully unfold on the silica surface. This may be explained by the fact the BSA molecule has a fixed three-dimensional structure and, probably, in this conformation, it is mainly sorbed on the silica surface. Thus the total area of the BSA monolayer projection in globular conformations is about 266 m^2/g, which does not exceed the value of the specific surface of high disperse silica. It was calculated that there are 4.4 adsorbed BSA macromolecules per one primary particle of the silica in this case. In the IR spectra of silica, a decrease in the intensity of the absorption band of free silanol groups (3750 cm^{-1}) is observed with an increase in BSA adsorption, and upon reaching a monolayer coating the OH-group is practically absent (Fig.). This indicates that all free silanol groups of the surface are involved in the interaction with BSA macromolecules. Using thermal vacuum studies, it was shown that the absorption bands with a maximum of about 3400 cm^{-1} are reduced when heated silica samples with adsorbed BSA. This means the physically sorbed water is removed from the surface in this condition. However, the absorption band of 3750 cm^{-1} is absent in the IR spectra of the samples even after heating to 290°C.

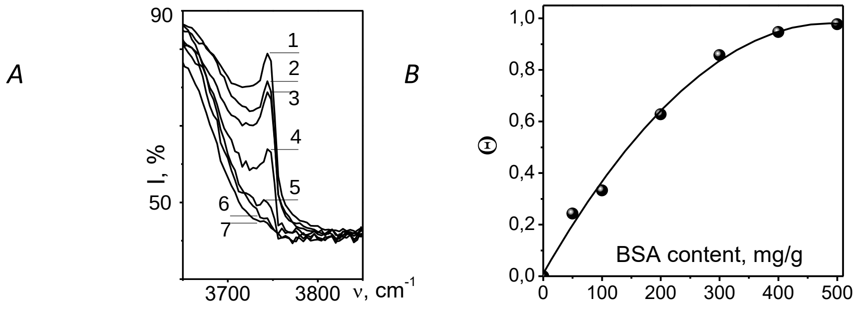

Fig. *A* - IR spectra of the silica (*1*) after 50 (*2*), 100 (*3*), 200 (*4*), 300 (*5*), 400 (*6*), 500 mg/g (*7*) BSA adsorption. *B* - The perturbation degree of OH-groups as a function of BSA content

Low-cost sorbents for the adsorption of pharmaceuticals

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Pharmaceuticals are toxicological contaminants of the aquatic environment. Removal of pharmaceutical from the wastewaters before discharge is a necessary conditions for cleaner production. Adsorption is a promising method for wastewater purification due to numerical advantages such as low energy consumption and simplicity of the operational parameters. Low-cost sorbents, e.g. prepared agricultural wastes, can be used for these purposes.

The aim of this study was to evaluate the sorption properties of lignin (L), cellulose (C) and lignocelluloses (LC) sorbents derived from sugarcane bagasse and straw towards sodium diclofenac. The hydrolysis of starting material with mineral and organic acids and delignification with hydrogen peroxide were used to obtain L-, LC- and C-sorbents. The characteristics of the resulting materials are given in Table 1.

Table 1. Structural properties

Indicator	Sugarcane bagasse				Sugarcane straw			
	Initial	L	C	LC	Initial	L	C	LC
Lignin/cellulose content, %	21.4/ 42.1	90.5/ 3	3.03/ 67.3	29/ 34.3	19.6/ 37.2	81.8/ 1	8.6/ 57.5	27.7/ 30.3
Specific surface area, m^2/g	1.35	2.98	1.25	1.23	1.93	6.68	5.37	2.68
Adsorption pore volume, cm^3/g	0.08	0.19	0.15	0.11	0.05	0.24	0.13	0.18

The sorption ability of biopolymers from sugarcane residues towards sodium diclofenac was investigated and the results are shown in Table 2.

Table 2. Sorption properties

Indicator	Sugarcane bagasse			Sugarcane straw		
	L	C	LC	L	C	LC
Efficiency of sodium diclofenac sorption, %	36.5	15.6	2.13	85.8	21.5	44.4

The values of sodium diclofenac sorption efficiency correlate with the values of the specific surface area and pore volume.

Our results demonstrate that sugarcane residues could be a promising source of biosorbents for water treatment from pharmaceuticals.

Aggregation processes in multicomponent nanosystems

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Nowadays cancer is the second leading cause of death after heart disease. Many traditional anticancer drug treatments exhibit limited efficacy and cause high morbidity. Combined therapy referring to the co-delivery of two or more therapeutic agents or a combination of different treatments is becoming more popular in clinical treatment of cancer because it generates synergistic anti-cancer effects, reduces individual drug-related toxicity and suppresses multi-drug resistance through different mechanisms of action.

Our recent research shows that *in vitro* experiments on malignant cell line MT-4 nanocomposite consisting of gold nanoparticles, photosensitizer chlorin e6 (Ce6) into dextran-graft-polyacrylamide matrix demonstrated twofold increase of photodynamic efficacy compared to the free photosensitizer [1]. Also it was reported that water-soluble star-like copolymer loaded by Doxorubicin (Dox) sharply decreased the viability of HeLa cells at the low concentrations [2]. Therefore, the idea was to create nanocomposite for complex photodynamic and chemotherapy, namely to synthesize polymer-based nanocomposite loaded by AuNPs, photosensitizer Ce6 and anticancer drug Doxorubicin simultaneously. However, it is quite complicated to predict the behavior of multicomponent nanosystems, because adding any component can cause aggregation processes, and lead to loss of biological activity of nanocomposite.

Consequently, this study was devoted to understand processes occurring during the formation of multicomponent nanosystem, which can be used for combined cancer chemo-photothermal therapy with increased efficacy. Thus, we investigated processes occurring in binary nanosystems Polymer/AuNPs, Polymer/Ce6, Polymer/Dox; ternary nanosystems Polymer/AuNPs/Ce6, Polymer/AuNPs/Dox, and 4-component nanosystem Polymer/AuNPs/Ce6/Dox. It was shown that aggregation processes are more significant for four-component nanosystem, and it is more reasonable to use Polymer/AuNPs/Ce6 and Polymer/AuNPs/Dox nanosystems consistently for complex photodynamic and chemotherapy.

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Simulation of optical spectra of structures with silicon nanowires

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In spite of the great achievements, reducing costs and improving the efficiency of solar cells will always be two major tasks in this area.

The use of ultra-thin c-Si films in the thickness of several microns can reduce the cost of the solar module. However, there is a problem that is accompanied by a decrease in thickness. It consists of insufficient absorption of the spectrum of solar radiation in the near infrared region. Thus, the widespread introduction of ultrathin c-Si for future solar cells primarily depends on new methods for improving the absorption of light. To increase the efficiency of solar absorption, solar cells with different nanostructures on the substrate surface began to be widely studied. Such nanostructures can be arrays of nanowires (Fig. 1).

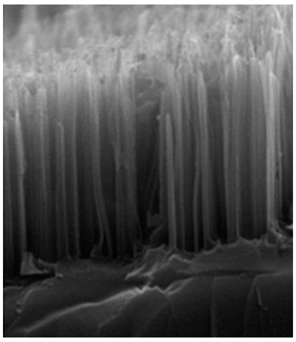

Fig. 1. SEM image of obtained cross section view of Si NWs [1]

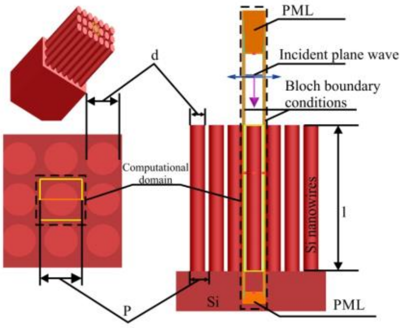

Fig. 2. Cross section of the simulation model

To obtain optimal forms, sizes and other parameters of nanostructure arrays it is necessary to conduct a lot of experimental research, which will cause a lot of difficulties. Therefore, in order to optimize the research work, it is expedient to use theoretical calculations at the first stage, which can then be verified experimentally. The tool for such researches is a time-domain finite difference (FDTD) method (Fig. 2) by which one can solve the Maxwell equation and obtain optical spectra of the investigated structures.

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The new reinforcement technology of concrete as the new percolation problem

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The report contains a brief description of the new reinforcementing technology of concrete by a mixture of steel powder and fiber, and also by areas of concrete with increased strength, which appear in places of contact with metal [1]. The feature of the technology is the creation in concrete of connected regions of percolation type, consisting of clusters of steel fiber and powder, which, at a critical concentration, cause an abrupt change of number parameters of material.

The computer percolation model of a reinforcing structural phase transition in dispersion-reinforced concretes has been developed for study the structure and properties of the obtained material.

In the model, the continual percolation problem of clusters consisting of quasi-point and quasilinear elements was solved for the first time. The problem is solved by the Monte Carlo method in a cube with a size of 10^6 units. Single fibers and powder particles in a model are considered to be connected, if they have a common point or the distance between them does not exceed a certain pre-set, which plays the role of a control parameter in the model. This distance plays the role of a control parameter in the model, as does the length of the fiber. Another parameter of the model is the powder particle diameter.

In addition, reinforcementing of concrete with metal filler, the model considers the possibility of increasing the strength due to mechanical stresses arising at the places of contact of concrete with fiber and powder. A criterion is obtained for the occurrence of such stresses under conditions of a decrease in the volume of concrete during hydration. The observed effects, in our opinion, demonstrates the similarity with the long-range effect in semiconductors and metals [2, 3].

The report describes the difficulties of the model due to the hyper-random nature of the values some parameters arising in the study.

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Conversion of *D*-fructose into ethyl lactate over SnO_2/Al_2O_3 catalyst synthesized by different methods

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In this communication the results on preparation of an effective catalyst for obtaining ethyl lactate from fructose as renewable raw material are presented. The SnO_2-containing alumina samples were prepared by incipient wetness impregnation (SnAl-imp), co-precipitation (SnAl-co) and mechanochemical activation (SnAl-mcho). All samples were studied using several techniques for determination of their structural, textural, and acid properties.

The X-ray analysis shows that no crystalline SnO_2 species could be detected for samples synthesized by co-precipitation and impregnation methods. Intense and narrow characteristic peaks corresponding to tetragonal SnO_2 for samples synthesized by mechanochemical method were detected.

UV–vis spectrum of SnAl-mcho sample shows a broad line around 260 nm that attributed to octahedral $^{VI}Sn^{4+}$ ions in SnO_2 phase. However, for SnAl-co and SnAl-imp samples the maximum intensity is observed at 215 nm that corresponded to isolated tetrahedral $^{IV}Sn^{4+}$ ions.

According to the titration results, all samples are weakly acidic oxides with $H_0 \leq +1.5$.

The transformation of 13% fructose solution in 98% ethanol over different SnO_2/Al_2O_3 samples was studied using autoclave rotated with 60 rpm at 160°C for 3 h. For oxides obtained by mechanochemical activation 90% conversion of fructose occurs with 5-hydroxymethylfurfural formation. The same effect is observed for pure SnO_2. It was found, that supported and co-precipitated SnO_2/Al_2O_3 catalysts provide 95-100% conversion of 13% fructose solution in ethanol with 50% selectivity towards ethyl lactate. At that, for SnAl-co and SnAl-imp samples leaching of tin oxide is not observed and they can be reused after regeneration at 500°C.

Porosity and structure peculiarities of POSS-containing nanocomposites based on PU/PHPMA semi-IPNs

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The impact of different amount of the 1, 2-propanediolisobutyl-POSS (1-10 wt. %) on the porosity and morphology of nanocomposites based on semi-interpenetrating polymer networks (semi-IPNs) of the crosslinked polyurethane (PU) and linear poly(hydroxypropyl methacrylate) (PHPMA) have been investigated. Semi-IPN15 and semi-IPN30 (PU/PHPMA=85/15 and 70/30, consequently) were used as matrix.

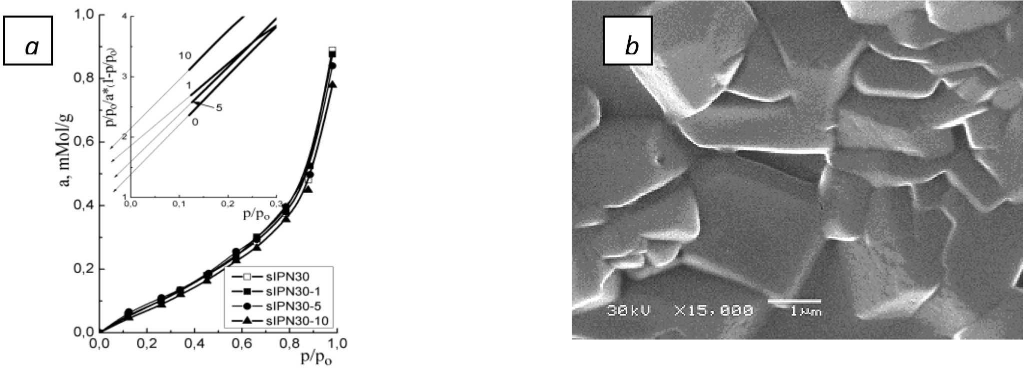

Fig. The isotherms of methanol vapour adsorption for semi-IPN30 matrix and semi-IPN30 nanocomposites with different POSS content (1-10 wt. %) (*a*); cross-sectional SEM images of semi-IPN30-5 nanocomposite (*b*)

The adsorption of methanol vapour by the nanocomposites was investigated by using of vacuum installation with McBean balances (Fig., *a*). The porosity, specific surface and average dimension of pores were calculated. The introduction of POSS nanoparticles into semi-IPN30 matrix with amount of 5-10 wt. % leads to decreasing of specific surface and total volume of pores. The average dimensions of nanocomposite's pores were in range of 50-60 Å.

The morphology of the nanocomposites was investigated by SEM. The structure of semi-IPN15 is comparatively homogeneous, the semi-IPN30 matrix has the heterogeneity with size about 50 nm. The introduction of 1-3 wt. % of POSS into the matrix semi-IPN-30 results in formation of the nanodomains with size of 50-100 nm. Increasing amount of POSS up to 5-10 wt. % leads to formation of microdomains of 1-3 µm size (Fig., *b*). Obviously, the POSS introduced into the semi-IPN matrix on the stage of PU synthesis acts as nanostructuring agent in the system. The obtained materials with more dense structure are promising for application as gas barrier membranes.

Water dynamics near the surface of cellulose nanoparticles

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Cellulose nanoparticles are flexible for chemical modifications due to the network of hydrogen bonds on its surface. The modification of the surface may significantly change the properties of the nanoparticles increasing the compatibility with other materials.

In our research, cellulose nanoparticles were produced by two methods [1] giving cellulose nanocrystals (CNCs) and nanofibers (CNFs). In order to vary the hydrophobic-hydrophilic properties of the nanoparticles, the poly(N-isopropylacrylamide (PNIPAM) was used. The dynamics of water near the surface was investigated by measuring the dielectric relaxation of 4 aqueous suspensions of CNCs, CNFs, CNCs+PNIPAM, CNFs+PNIPAM.

The calculated relaxation time (Fig.) indicates that the addition of the CNFs slows down the dynamics of hydrogen bonds, however, the addition of CNCs do not affect the dynamics significantly. The addition of the PNIPAM slows down the dynamics of both samples.

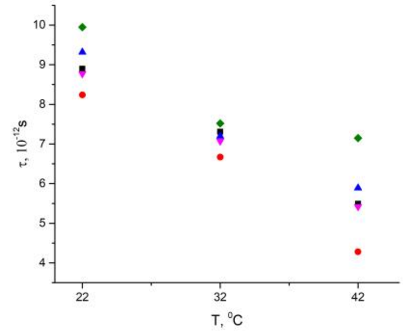

Fig. The temperature dependence of the relaxation time of water (■), CNCs (●), CNFs (▼), CNCs+PNIPAM (▲), CNFs+PNIPAM (♦)

This result is explained by the possibility of two variants of structural and geometric changes in the hydration layer near the hydrophilic surface, as consequence, the relaxation time can be either greater or less than that of water, however, the hydrophobic surface only increases the relaxation time [2].

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Design and characterization of SERS substrates

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Surface-enhanced Raman spectroscopy (SERS) is effective, fast growing analytical method which finds a lot of applications in chemistry, medicine, pharmacology, ecology *etc*. [1]. SERS allows study of ultralow concentrations, up to single molecule detection of different substances. One of prerequisites of effective application of SERS is placement of the target molecules near a metal nanostructure, because electrical field from surface plasmons decreases exponentially with distance. Depending on electrical charge of molecule and state of metal surface, it can be possible also chemical bonding between them to be realized. SERS effect sufficiently depends also on the morphology of nanostructures, conditions of molecule deposition, and parameters of laser excitation. Therefore, it is necessary to design SERS substrates based on nanostructured gold or silver, which would be stable in time, simple in preparation, and effectively enhancing Raman signal of various substances.

In this work, relatively inexpensive and simple in the fabrication SERS substrates based on gold and silver nanoparticles (NP) obtained by the method of colloidal chemistry [2] have been developed. Namely, the core-shell nanostructures: SiO_2-Au, Au-SiO_2, star-like and bimetallic (Au, Ag) NP. Using of alloys of bimetallic it is allows expand working area of plasmon substrates to the range of 400 nm.

Surface morphology of fabricated SERS substrates was investigated by scanning electron microscopy, optical and Raman spectroscopy. The position of maximum of surface plasmon resonance was defined for each type of substrate. It is shown that by using bimetallic nanostructures it is possible to change gradually the position of plasmon maximum. The star-like NPs are found to have two maxima of plasmon absorption in visible and IR. Enhancement of Raman signal of low concentration of crystal violet molecules was obtained for each of prepared SERS substrates.

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Photodegradation of 4-nitrophenol in presence of mesoporous Au/TiO_2 and Cu/TiO_2 films

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Titania is well known and active photocatalyst in the redox processes of mineralization and degradation of many environmental pollutants. Nitrogen-containing phenols are very toxic pollutants witch give rise to serious health problems. In recent years, addition of transition metal ions has been observed to increase the rate of TiO_2 photocatalytic degradation of organic pollutants because to the role of the metal ions as electron scavangers.

In this paper, we present the results of comparative study of 4-nitrophenol (4-NP) photodegradation in presence of thin mesoporous TiO_2 and TiO_2/Au and TiO_2/Cu films. TiO_2/Cu porous films covered on a glass substrate were obtained by sol-gel method. Nonionic amphiphilic triblock copolymer Pluronic P123 was used as a template agent and acetylacetone as a complexing agent. The films were calcined at 130, 300 and 400 °C subsequently and show anatase structure. Pure nanocrystalline TiO_2 films have pore size radius around 5 nm.

Optical properties of synthesized films were characterized by UV-vis spectroscopy.

The results show that the photocatalytic degradation of 4-NP with the addition of Cu or gold ions results negative effect compare to pure TiO_2 film action. Under UV-irradiation TiO_2/Cu films, the reaction of photoreduction of Cu^{2+} to Cu^{1+} takes place. Low photocatalytic activity may be attributed to the low reduction potential for Cu^{2+}/Cu^{1+} couple. Therefore, as a result, there is no formation of $OH^{\cdot}$ radicals, which are the main factor of photocatalytic action. Similar results were obtained in the aqueous water suspensions of titania contained Cu^{2+} ions in the work [1]. Thus, we may conclude that Cu^{2+} has an inhibitory effect on the photodegradation of 4-NP.

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The effect of substrate temperature and air annealing on the structure, optical and electrical properties of MoO_x thin films deposited by reactive ion-beam sputtering

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In recent years, molybdenum oxide (MoO_3 with bandgap about 3.3 eV at room temperature) films have attracted considerable attention due to their great potential application as an electron-blocking and hole-selective layer as well perspective buffer layer for fabrication cost-effective solar cells and light emitting diodes [1].

In our report, we at the first time examine the reactive ion-beam sputtering (RIBS) deposition method for the growth of MoO_3 films. RIBS was considered to be the most interesting growth method for deposition films due to a good films adhesion, high deposition rates, film uniformity of over large substrate areas and a very smooth surface of the deposited films, that is critically important for optoelectronic applications [2].

Our report devoted to investigation of the influence of substrate temperature in the range from the room temperature to 300 °C and air annealing on the structure, optical and electrical properties of MoO_x thin films deposited on Si and glass wafers by RIBS. X-ray diffraction, photoluminescence, Raman scattering, energy dispersive X-ray spectroscopy, multiangle spectroscopic ellipsometry, optical transmission and electrical measurements were used for samples characterization. It was found that the application of substrate temperature as well as post-growth air annealing allow us to sufficiently influence on the properties of MoO_x thin films. Obtained results will be analyzed and discussed.

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Effect of synthesis conditions on the catalytic activity of cobalt oxide in hydrogen peroxide decomposition

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This paper presents the results of a study of the relation between the synthesis conditions of nanoscale cobalt oxide, its spatial structure and catalytic properties, which are exhibited by this compound during hydrogen peroxide decomposition.

The samples were synthesized by the sol-gel method from cobalt(II) nitrate solutions using ammonia or hexamethylenetetramine (Hexa) solution as a precipitant. Obtained hydrated oxides were heat treated for 4-7 h at 80 °C and 2 h at 400 °C. X-ray investigations show the formation of a mixed Co_3O_4 oxide, whose average particle size was 6-15 nm, according to the Scherer equation.

The spatial organization of the particles of samples was studied by SEM. The particles of cobalt oxide precipitated with ammonia hydroxide are shaped as globules, formed by the coalescence of flat particles, and the samples obtained by using Hexa are composed of two-dimensional plates. Calcination at 400 °C leads to partial breakdown of two-dimensional structures. The characteristics of samples obtained under different conditions are listed in the Table.

Table. Surface characteristics of cobalt oxide

Synthesis conditions (precipitant) [temperature]	Specific surface area (m^2/g)	Pore volume (cm^3/g)	Pore size (Å)
(NH_3) [80 °C]	101.7	0.8435	165.8
(NH_3) [400 °C]	47.7	0.7935	332.7
(Hexa) [80 °C]	19.38	0.1523	157.2
(Hexa) [400 °C]	26.94	0.1986	147.4

The catalytic activity of synthesized samples in hydrogen peroxide decomposition was studied. It has been found that the samples dried at 80 °C have the best catalytic activity independent of synthesis conditions. The oxide samples synthesized by precipitation in a Hexa solution have an almost three times higher catalytic activity than the samples obtained by precipitation in ammonia hydroxide solution. Heat treatment for 2 h at 400 °C reduces the catalytic activity of samples both in the former and in the latter case.

The obtained results indicate that depending on synthesis and heat treatment conditions, the synthesized cobalt oxide samples have a different morphology, which, in turn, affects greatly their catalytic activity.

Disintegrating dosage forms for prolonged antioxidants release based on silica-gelatine matrix and orchids extracts

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Gelatine is known to be extensively used in pharmaceutical industry for the preparation of disintegrating dosage forms with prolonged drug release. In particular, such the forms may be prepared as the thin gelatine films with the active substances embedded in the polymer pores. Upon entry into aqueous medium, drug-containing gelatine films gradually swell and release the active ingredients. To provide the additional retardation of the drug release, one can use silica-gelatine materials instead of gelatine ones. Due to high concentration of $\equiv SiO^- / \equiv SiOH$ surface groups, silica strongly interacts with gelatine molecules acting as peculiar (but effective) cross-linking agent.

The aim of the work was to prepare and study the gelatine and silica-gelatine matrices with embedded antioxidants – the components of orchids extracts. Gelatine and silica-gelatine films with incorporated antioxidants molecules were prepared according to [1]; the extracts from the leaves of *Dendrobium nobile* Lindl. and *Anoectochilus formosanus* Hayata plants were used as bioactive ingredients. Composition and antioxidant properties of the extracts, swelling of the films and desorption of the extract components from the films into water was studied.

The extracts were found to contain significant amounts of phenol compounds (flavonoids, phenolic acids, *etc.*) and possess high antioxidant properties (total phenolic index of ~1). The addition of the extracts to gelatine/silica-gelatine films did not strongly affect the films properties, while the presence of silica in the films leaded to significant (by ~2 times) decrease in the film swelling. The deceleration of swelling of silica-gelatine films also resulted in a slower release of incorporated bioactive compounds: for 24 h of desorption, ~75 % of extracts components were released into water from gelatine films whereas only ~ 50 % of antioxidants were desorbed from silica-gelatine ones. Thus, the silica-gelatine films with embedded orchid extracts seem to be promising dosage forms for prolonged antioxidants release: the components of the extracts are effective natural antioxidants while silica-gelatine matrix provides their gradual release and prolonged action.

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Medical-preventive drug against iron deficiency anemia in animals

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An anti-stress, environmentally friendly anti-anemic drug with high bioavailability (biodegradability) and low toxicity was obtained, intended for oral use, and prospects for its use in the field of animal husbandry (namely, pig breeding) were determined. To obtain a drug with the above characteristics, a method has been developed for preparing a complex compound by reacting iron carbonate (the main active component is iron(II)) and cobalt chloride with the monosaccharide *D*-fructose, which has hemostimulating properties.

The drug is a complex mixture containing certain amounts of fructose Fe(II), fructose Co(II) and highly dispersed askan-clay (obtained by ultrasonic dispersion of an aqueous suspension). The solid form of the drug for oral administration, manufactured by the above method, contains (in mass %): Fe(II)-Fructose 15.75-31.6, [Fe(II)-3.75-7.5], Co(II)-Fructose 0.28, [Co(II)-0.07], natural Askan-clay 68.2-36.5. Therapeutic and preventive efficiency of manufactured preparation was tested on piglets under study, on pig's farms (toxicity of preparation was preliminary tested on laboratory white rats). Experiment result was expressed in getting rid of complications (iron deficiency anemia, diarrhea-dyspepsia) caused by stress factors related to termination of breast feeding of store piglets and food change, as well as in their normal growth and development, normal blood chemistry values and live weight gain (Table).

Table. Impact of the developed preparation on the increase in live weight of piglets (20-120 days)

Group	Pigs age, days					
	20	30	40	50	60	120
	live weight, kg					
I	4.50±0.20	7.30±0.25	9.55±0.40	13.22±2.42	16.85±2.29	100.20±3.50
II	4.90±0.30	7.80±0.35	9.80±0.45	13.58±2.50	17.3±2.40	102.0 ±3.10
III	4.00±0.30	6.80±0.40	8.00±0.45	12.50±2.45	15.80±2.50	98.45±2.80

I – preparation with 7.5-9.0% content of Fe(II), *n*=12; II – preparation with 3.75-7.5% content of Fe(II), *n*=12; III – control group, *n*=5

According to the data in the Table, the preparation with Fe(II) content of 3.75-7.5% is optimal.

Lower olefines obtaining over membrane composite catalysts

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One of the perspective way carbon dioxide utilisation is chemical conversion to useful materials. This direction is very attractive thus allow not only decrease global warming, which causes the concentration of atmospheric CO_2 to increase but propose a solution to substitute for the exhaustive fossil fuel. However, it's well known that carbon dioxide is a very stable molecule. This is the biggest barrier to commissioning CO_2 because it's transformation in need of a great deal of energy.

Taking into account our scientific experience in the field of catalysis, we propose to process carbon dioxide on composite membrane catalysts (Fig.).

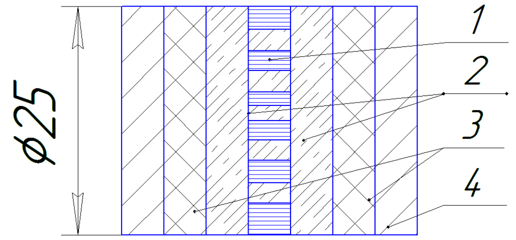

Fig. Principal scheme of membrane-catalytic composite:
1 – supporter; *2* – proton conductive material; *3* - catalytic component; *4* – lead

Our developed membranes are the complex of polyfunctional systems, which consist of several layers: proton-conductive and catalytic. This approach allows us to organise a one-stage process with selective production of lower olefins from a mixture of $CO_2 + H_2$. It was found that the use of compositions from already known bifunctional catalysts (copper-zinc, molybdenia-nickel-alumina, platinum-aluminium oxide, ferrum-containing), allows both carbon build-up and control of double bonds hydrogenation in this chain. It should be noted the role of proton-conductive material - the possibility of organising the hydrogen's transport to active centers in the form of protons with subsequent their recombination in atomic hydrogen. It is controlling the value of the proton current to provide the necessary concentration of active hydrogen on the surface of the catalyst involved in the process of hydrogenation. Hydrocarbons series from C_1 to C_5 with various hydrogen content in the carbon chain were obtained in testing the received membrane-catalytic composites.

Acknowledgements
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More on the size dependence of the high-frequency surface conductivity of achiral carbon nanotubes

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Over the past few decades, one of the most current tasks of the modern physics of the microwave frequency devices is the creation of reliable, portable, customized sources and sensitive detectors of terahertz radiation (THz). The usage of the carbon nanotubes (CNTs) as building blocks for high-frequency devices is one of the latest trends in the microwave frequency engineering. The question of the dimensional dependence of the real part of the surface conductivity of the microwave frequency single-layer CNTs remains underinvestigated.

The real part of the high-frequency surface conductivity is determined by the following equation [1]:

$$\mathrm{Re}\,\sigma_s(\omega) = -\frac{e^2}{2\pi^2 \mathrm{h}\tau R}\left(\frac{1}{\omega^2+\tau^{-2}}\mathcal{I}_1 + \frac{2\omega^2}{\mathrm{h}}\mathcal{I}_2\right) \qquad (1)$$

where ω is the frequency of the incident electromagnetic wave; τ is the relaxation time; R is the radius of CNTs;

$$\mathcal{I}_1 = \sum_{s=1}^{m}\int_{-a}^{a}\mathcal{F}(p,s)\,dp\,; \quad \mathcal{I}_2 = \sum_{s=1}^{m}\int_{-a}^{a}\left(\omega_{\mathrm{cv}}^2(p,s)-\omega^2+\tau^{-2}\right)\mathcal{F}(p,s)\,dp\,; \qquad (2)$$

$$\mathcal{F}(p,s) = \frac{1+\cos\frac{3bp}{2\mathrm{h}}\cos\frac{\pi s}{m} - 2\cos^2\frac{\pi s}{m}}{\left[\left(\omega_{\mathrm{cv}}^2(p,s)-\omega^2+\tau^{-2}\right)+4\omega^2\tau^{-2}\right]\varepsilon_c^3(p,s)}\,\mathrm{th}\left(\frac{\varepsilon_{\mathrm{c}}(p,s)}{2k_{\mathrm{B}}T}\right), \qquad (3)$$

where m, n are the chirality indexes; $b = 0{,}142$ nm is the interatomic spacing in the graphene crystalline lattice; T is the temperature of the electronic subsystem of a carbon nanotube; p is the quasi-impulse of the electrons; $\varepsilon_c(p,s) = \mathrm{h}\omega_{cv}(p,s)$, $\omega_{cv}(p,s)$ is the frequency of the interband transitions.

The results of the calculations of the dependence of the dimensional dependence $\mathrm{Re}\,\sigma_s$ have shown that due to the discrete change in the chirality of the curves $\mathrm{Re}\,\sigma_s(R)$, the formation of the sharp peaks occurs. At the same time with the small m value number, the oscillations $\mathrm{Re}\,\sigma_s(R)$ have a large amplitude of chirality, which decreases when m increases.

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Effect of quercetin on the swelling behaviour of silica-gelatine matrices for prolonged antioxidants release

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Flavonoids are effective antioxidants widely used in pharmacology. In particular, these antioxidants may be used in disintegrating dosage forms with prolonged drug release. Gelatine/silica-gelatine matrices with embedded bioactive substances are the examples of such the forms; upon entry into water, such the matrices gradually swell and release the active ingredients. The embedded substances by themselves may affect the silica-gelatine and gelatine-gelatine interactions, either retarding or accelerating the matrices swelling.

The aim of the work was to study the effect of quercetin on the swelling behaviour of gelatine and silica-gelatine matrices. The matrices were prepared in the form of thin films according to [1], with 1 mM solution of quercetin being used to incorporate the flavonoid in the films. The PM7 method and the COSMO solvation model implemented in the MOPAC2016 software package were used for quantum-chemical modelling of supramolecule complexes.

Fig. shows that addition of the flavonoid to gelatine films does not strongly affect the film properties, while the presence of quercetin in silica-gelatine film leads to notable (~15 %) increase in the film swelling. The values of Gibbs free energies of interaction Δ*G* (Table) show that quercetin forms weaker hydrogen bonds with gelatine molecules than with silica surface groups.

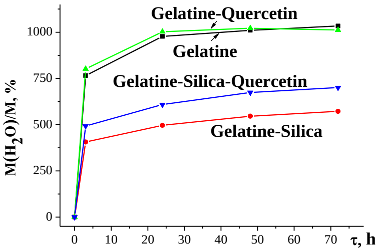

Fig. Swelling of the films

Table. The values of Gibbs free energies of interaction Δ*G* of quercetin with gelatine molecule (fragment) and silica surface groups

System	-Δ*G*, kJ/mol
Quercetin - Gelatine	16
Quercetin - Silica	28
Gelatine - Silica	54

Thus, quercetin was not found to be cross-linking agent for gelatine materials, as it was stated in [2]. The effect of quercetin on the properties of silica-gelatine matrices seems to be the result of silica-quercetin interaction rather than quercetin-gelatine interaction. One may conclude that the adsorption of quercetin on the silica surface leads to screening of the part of silica silanol groups from gelatine molecules and, therefore, to the weakening of silica-gelatine interaction.

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Synthesis of pH-sensitive magnetite-laponite nanocomposite

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In order to create matrices for controlled release of biologically active compounds, there is a need to create non-toxic nanocomposite hydrogels for biomedical applications with increased biocompatibility and bioavailability [1]. Traditionally hydrogels are synthesized by chemical crosslinking of monomers, using N,N′-methylenebisacrylamide. This method has some disadvantages that limit application of such hydrogels. To avoid this, a synthesis method based on the physical crosslinking of a copolymer using to laponite nanoparticles is applied [2]. The effectiveness and targeting of drug release could be greatly improved by using magnetic nanoparticles, since the chemotherapeutic agents attached to them concentrated in the immediate proximity to the target organ by applying an external magnetic field. pH-sensitive hydrogels with carboxyl or amine functional groups for drug binding to a polymeric matrix due to selective sorption has created much interest for drug delivery systems.

Synthesis of pH-sensitive hydrogels composites based on acrylic acid and laponite was carried out (the schematic representation shown below in Fig.). Laponite was dispersed using a magnetic stirring, sodium dodecyl sulfate were added, and then placed in an ice bath, and acrylic acid and ammonium persulfate were added. The mixture was placed to a test tube and heated at 50°C for 10 h.

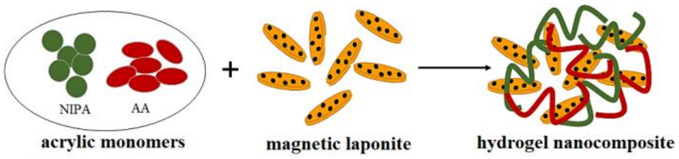

Fig. Schematic diagram for the synthesis of hydrogel nanocomposite based on magnetite-laponite

Hence, based on magnetite-laponite nanoparticles, physically-crosslinked pH-sensitive nanocomposites with improved mechanical properties and ability to phase transitions (swalling–collapse) by changing from neutral to slightly acidic pH have been synthesised.

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Photocatalytic degradation of dyes using phosphorus-containing active carbons

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The nature and mechanism of the photocatalytic activity of carbon materials are actively studied [1, 2]. Particularly, it was shown that introduction of oxygen heteroatoms and cations of transition metals into the structure of active carbon (AC) improves its photocatalytic activity [3]. In this communication, photodegradation of dyes using phosphorus-containing AC doped with copper and cobalt (about 1.5% of P and 0.5% of metal ions according to XPS data) under visible illumination is reported. Phosphorus-containing AC has micro-mesoporous structure (fraction of mesopores is 19%), specific surface area 783 m^2/g and content of acid surface groups 1.904 mmol/g. Cu- and Co-doped carbons were prepared by impregnating of phosphorus-containing carbon with metal nitrates solutions at pH=3, washing with distilled water and drying. Metals obviously occupy cation exchange positions in phosphate groups with pK=2.

Initial phosphorus-containing sample shows activity in rhodamine B (RhB) and safranin T (ST) photodegradation under visible irradiation although pristine AC sample without phosphorus was inactive in the same conditions [3]. This can be associated with the presence of phosphorus heteroatom in the structure of AC, which causes narrowing of band gap [1]. Phosphorus-containing AC is more active compared with phosphorus-free AC despite the fact that its specific surface area is 20% lower, and the photocatalytic testing was conducted not in the form of disperse powder, but in the form of granules with size of 0.6 mm. The latter makes it easy to separate the photocatalyst from the liquid phase and reuse it three times practically without loss of activity. The degree of dyes decolorization for these catalysts is 80-90% for 3 h but mineralization is only 63-73% (according to TOC measurements).

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Photoinduced synthesis of Ag(Au)/tryptophan nanoparticles by UV-C LEDs sources

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The Ag(Au)/tryptophan systems [1] are the promising bases for design of hybrid biocompatible silver(gold) nanoparticles Ag(Au) NPs and its further implementation in cancer diagnostics and therapy. The physical and chemical properties of such system depend on the size of Ag(Au) NPs. However, the size-controllable process of formation of Ag(Au) nanoparticles in the presence of amino acid tryptophan is still unclear. We assume that morphology of synthetized Ag(Au) NPs can be controlled by two ways: chemical and photochemical.

The novel deep ultraviolet (UV-C) light emission diodes (LED), which are currently available on a market, are advantageous source for photochemical synthesis of metal-based nanoparticles. Therefore, we can affect the rate of reaction with further control of the resulting characteristics of nanobjects (e.g. optical properties, size, and morphology) using different parameters of UV irradiation (e.g., wavelength, optical power density, duration) of UV irradiation of the reaction mixture.

For comprehensive analysis of the photoinduced kinetics [2,3] the portable experimental setup with series of UV LED sources was developed. For the photochemical activation of Ag(Au)/Trp systems, we applied UV-C LED source (LGInnotek) with the wavelength of $\lambda = 278$ nm at output optical power density of $P = 1.0\pm0.1$ mW/cm^2.

The present study is focused on photoinduced processes in Ag(Au)/Trp system. At the same time, our investigation aimed to control the NPs optical properties and morphology as the key factor determining their resulting characteristics.

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Sorption of Cd^{2+} ions on nanosized zero-valent iron/kaolinite composite

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The problem of water purification from heavy metals it is one of the most insistent problems that require innovative solutions. Cadmium is one of the most toxic heavy metals, classified as high-risk substances. Cadmium has a certain tendency to accumulate in the human body, specifically in the kidneys and liver. Cadmium enters natural waters due to anthropogenic activities, as cadmium is a widely used element for the production of anti-corrosion coatings, electrodes and pigments.

For today cadmium from natural waters is removed by applying classical methods – chemical deposition, membrane filtration and a group of adsorption methods.

The newest sorption material is nanoscale zero-valent iron (n-ZVI), which demonstrates the high ability to remove heavy metal ions from aqueous solutions due to a complex sorption-reducing mechanism. The main problem of n-ZVI is the propensity to aggregate particles. The reason it is agglomerated ZVI particles are not transportable nor deliverable, well then cannot be used for *in situ* applications. Several methods have been proposed to solve this problem by using some solid matrix (resins, porous carbons, polymers). Kaolinite as a low cost widespread clay may be perspective solid matrices for immobilization of nanoscale ZVI.

The aim of this work was to synthesize and characterize kaolinite-supported nanoscale ZVI and to test it for the removal Cd^{2+} from aqueous solutions. The natural kaolinite was used to support nanoscale iron particles. The synthesis of n-ZVI was conducted using $FeCl_3 \cdot 6H_2O$ and $NaBH_4$ as reductant in water kaolinite dispersion. Mass ratio between the components of nanocomposite materials was 0.1 : 1.

The value of adsorption for kaolinite-supported n-ZVI is more than 15-20 times than for natural kaolinite, the maximum value adsorption reached 8.0 mg/g. The process of sorption on a kaolinite-supported n-ZVI does not depend on the value of the pH solution. The equilibrium concentration of Cd^{2+} is established at 15 minutes of contact with n-ZVI.

The obtained composite sorbent demonstrated the high ability of the for removal cadmium from solutions, according to the results.

Synthesis, structure and morphology of alkali metal titanates

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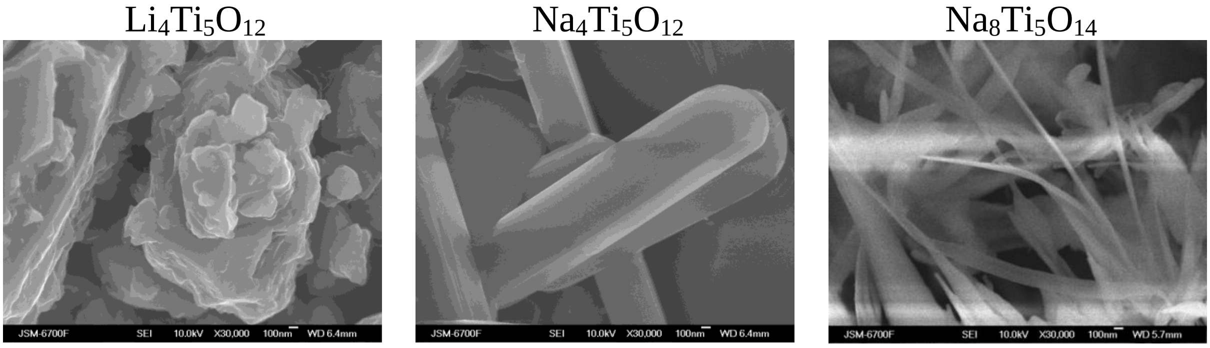
Secondary batteries are now the most widely used autonomous power sources. Some of them contain alkali metal titanates as negative electrodes. Stable operation of batteries requires homogeneity and crystallinity of electrode materials and significantly depends on the method of their synthesis.

In this communication, we aim at the study of the influence of temperature and residence time on the morphology of $Li_4Ti_5O_{12}$, $Na_4Ti_5O_{12}$ and $Na_8Ti_5O_{14}$ sintered from titania and lithium (sodium) carbonate.

Firing has been performed at 800-1000 °C for 6-60 h. In order to homogenize the samples, they have been grinded each 6 h. So as to optimize the process conditions and to obtain single, well-crystallized and homogeneous samples, their structure and composition has been determined by means of X-ray diffraction.

The particle size and morphology of the synthesized materials have been analyzed on a scanning electron microscope. In Fig., we compare $Li_4Ti_5O_{12}$, $Na_4Ti_5O_{12}$ and $Na_8Ti_5O_{14}$ obtained at the best experimental conditions, i.e. firing at 850 °C for 36 h.



$Li_4Ti_5O_{12}$ $Na_4Ti_5O_{12}$ $Na_8Ti_5O_{14}$

Fig. Scanning electron micrographs of alkali metal titanates obtained at the same magnification

Model systems for bioremediation of the water containing the mixture of hydrophilic and hydrophobic silica and bacterial cultures

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Today the urgent problem in many countries of the world is the pollution of the environment by anthropogenic origin substances, which include the oil and petroleum products (gasoline, diesel fuel, lubricants, fuel oil) that can form the toxic compounds which penetrate into the water and the soil [1, 2]. The most progressive method of water purification from hydrocarbons is the bioremediation – the process, aimed at returning of the contaminated environment to its natural state by using the microorganisms (bacteria and fungi) [2]. This method can be applied by immobilizing the microorganisms on the surface of the dispersed mineral carriers, in particular, the pyrogenic silica. Therefore, the purpose of the work was to create a biocomposite system for the destruction of the motor oil hydrocarbons, based on the mixture of hydrophilic (A-300) and hydrophobic (AM1-300) silicas and several types of bacteria of the *Bacillus* genus, which are the part of the biopreparation („Dr. Robik 106", Ukraine). The A-300:AM1-300 original ratio was 1:1, and the mixtures of silica to cells was 1:0.5; 1:1; 1:2.

As a result of the model study, it was found that for the sample with the highest content of the mixtures of silica, the complete disappearance of the oil film was observed in 14 days, and the presence of the secondary microflora was not observed even after 5 months of the experiment. At the same time, for the samples in which were present the bacteria *Bacillus* only (without silica), the secondary microflora was detected by the 20th day of the experiment. It means that silica actively promotes the activity of the microorganisms, presumably, by increasing the permeability of the cell membranes for nutrients and products of the cellular metabolism. It was established that the adsorption of the motor oil by the mineral composite is proportional to its amount, and the presence of bacteria in the composition of the composite system reduces its addictive capability. Compared to the pure culture of the biopreparation, the utilization of the motor oil by the biocomposite is much more efficient. That is, the proposed system can be recommended for the practical application.

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Magnetic composites based on activated carbon impregnated with pectin, polyethyleneimine and metal ions: antibacterial and adsorption properties

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The present research is devoted to study the adsorption behaviour of magnetic composites based on activated carbon (AC) impregnated with crosslinked polyethyleneimine (PEI) and magnetite as multi-purpose adsorbent towards organic, inorganic and bacterial contaminations (model objects: methyl orange (MO), metal ions, gram-positive and gram-negative bacteria) from aqueous solution. The composites were prepared by two approaches. In the first one materials were prepared by means of solid state dispersion method using AC, magnetite and pectin-PEI (1:2, protonated by 0.1 M HCl) at various weight ratios. By the second one crosslinking PEI was carried out on the AC surface. The interaction between pectin and polyethyleneimine is due to saponification of pectin's ester group and leads to the formation of crosslinked and insoluble product (pectin-PEI) [1]. As results we obtained composites containing 10-45 wt% of Pectin-PEI, 10-80 wt% of AC and 10 wt% of Fe_3O_4 [2]. The main components of the prepared composites which provided high adsorption capacity towards MO is protonated forms of pectin-PEI or its complexes with metal ions Zn^{2+}, Cu^{2+}, Pb^{2+}, Hg^{2+}, Fe^{3+} in an amount of 0.6-1.6 mmol/g. The adsorption capacity increased (up to 1123 mg/g) with increasing pectin-PEI content from 10 to 45 wt% for protonated components. The adsorption mechanism of MO is explained by ionic exchange or formation of a coordination bond between the sulfo group of MO and metal ions. By the way, for composites containing metal complexes adsorption capacity are also high (300-700 mg/g). The adsortpion kinetics of MO on magnetic composite was reached after 4-60 minutes and depending on the concentration of MO (15-700 mg/L) in solution. In aditionally, the antimicrobial activity was investigated against gram-positive bacteria (*Rhodococcus erythropolis*, *Bacillus subtilis)* and gram-negative bacteria (*Pseudomonas pseudoalcaligenes*, *Pseudomonas aeruginosa)* for sample which simultaneously containing 1-3.5 wt% of Ag, Zn and Cu nanoparticles [3].

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Binary mixtures adsorption of cationic and non-ionic surfactants

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In this paper, the adsorption of hexadecylpyridinium bromide (HDPB) and octylphenol ethoxylates of the TX series (TX-45, TX-100 and TX-305) from their mixed solutions on the graphitized carbon black (CB) was studied for determining the mixed adsorption main features of cationic and non-ionic surfactants on the nonpolar solid surface. This study aims to promote a better understanding of the surfactants interaction on the surface of a hydrophobic sorbent to optimize such interactions.

The specific surface area of the graphitized CB evaluated by BET method with argon adsorption was 105 m^2/g. Mixed HDPB – TX systems have been studied over a concentration range of (1.5-5.0) 10^{-5} mol/dm^3. The molar fraction of TX (α_{TX}) in the solutions were 0.2, 0.4, 0.6 and 0.8, respectively. The surfactants mixtures were investigated at pH 6.0-6.5 and at constant ionic strength of the solution. The concentrations of TX and HDS in the probes were determined by the spectrophotometric and two-phase titration methods, respectively.

Adsorption isoterms of the individual surfactants and their binary mixtures on graphitized CB were obtained. The composition of the mixed adsorption layer on CB surface was calculated using the Ruben-Rosen theory and this composition agrees with the experimental data. The regularities of change in surface activity of surfactant mixtures at the liquid - solid sorbent interface correlate with those for the liquid-air system with the increase in the total concentration of surfactants in solution, but are more pronounced.

The results of studies show that the surfactant composition on the CB surface is significantly different from their composition in the solution. A synergistic effect was found for surfactant mixtures when the adsorption of both non-ionic and cationic surfactants on the CB surface with their binary mixtures was higher than surfactants adsorption from individual solutions. It is shown that the parameters of β^σ intermolecular interaction, which are calculated using the Rubin-Rosen approach, have negative values indicating the presence of significant intermolecular interactions of the components in the mixed adsorption layer. It is shown that non-ionic surfactant molecules are dominant in the mixed adsorption layer. It is established that the molar fraction of non-ionic surfactants on the CB surface decreases in TX-45> TX-100> TX-305 series. These data indicate that more hydrophobic non-ionic surfactant is adsorbed predominantly on the CB surface from mixed solutions with cationic HDPB.

Structural features of phthalonitrile nanocomposite and their thermal destruction

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Phthalonitrile nanocomposites with amine-montmorillonite and A-300 silica nanoparticles at filler content of $C \leq 1\%$ were investigated by thermal analysis and temperature-programmable desorption mass spectrometry.

It is established the structure of pristine polymer and its composites includes two different structures, one of which decomposes in temperature range of 400-550 °C with a thermal destruction mechanism, and the second one thermally destroys in the interval of 550-800 °C with a thermo-oxidative mechanism. Atomic spectra of thermal destruction fragments for the low and high temperature structures show a significant difference in their atomic structure (Fig.). The thermal decomposition products for the first structure are the fragments of benzene ring C_6H_5OH (*m/z* 94), which confirm the aromatic polymer nature. In the decomposition spectrum of second structure the nitrogen-containing fragments as $OCNH_2$ (*m/z* 44) and NH_4 (*m/z* 18) take place. They may arise during the destruction of isoindoline, triazine and phthalocyanine heterocycles. Besides, the intensive thermal destruction for high-temperature structure at temperatures $T \geq 350\,^{\circ}C$ is stimulated under thermal decomposition in a vacuum for the composites with amine-montmorillonite nanoparticles. The pristine polymer and its nanocomposites decompose at temperatures of 450-570 °C under heat treatment in an air. Thus, thermal decomposition of materials in vacuum and in the air occurs with oxygen participation.

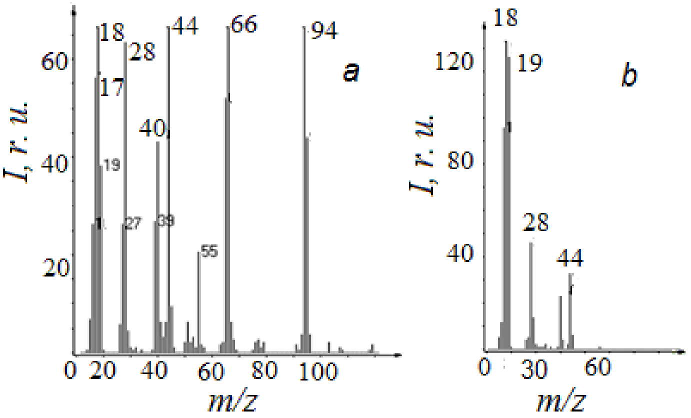

Fig. Mass spectra of low temperature (*a*) and high temperature (*b*) structures

Influence of nanodisperse metal on viscoelastic and thermophysical properties of polyvinylchloride

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The influence of surface and content of copper (Cu) nanodispersed powder obtained by the physical-chemical method (ph/c) and the method of electric explosion of the conductor (EEC) on the properties of polyvinylchloride (PVC) has been investigated. On the basis of the proposed model, the calculation and analysis of the structure of the surface layers (SL) Cu structures were made, the effective characteristics of the oxide film (OF) were determined, the dynamics of their changes was investigated, depending on the curvature of the surface of the nanoparticles (the mode of formation), the conditions of the environment. The volumetric content (φ) of Cu as a filler of PVC (KSR-676 MM 1,4·105) was $0 \leq \varphi \leq 5.0$ vol. %, temperature (T) range of studies 298 K$\leq T \leq$353 K, time (τ) of the presence of nanodispersed powder in the atmosphere at p = (746÷758) mm Hg, T = 303 K, humidity φ_B = 63% was $0 \leq \tau \leq 144$ h. It is established that the value of the time-weight gradient $(\partial p/\partial \tau)_{T,\varphi}$ is nonlinearly decreasing, indicating the aspiration of OF to quasi-equilibrium state. It is shown that the values: volume (V_0); density (ρ); the volumetric content (φ_{of}) of OFs is nonlinear in dependence on the type (ph/c and/or EEC) and the content of nanodispersed metal in PVC. Using the statistical approach to the analysis of the structure of PVC, taking into account the inter-intramolecular interaction, as well as the side groups (H, Cl) with the active centers of the surface of the filler in the donor-acceptor mechanism, the value of the anharmonicity factor (α) and the frequency variation (ν_i) of the oscillations structure formation. It has been shown that ν_i= f (T, φ, ph/c, EEC) causes the change in free energy (F), entropy (S), heat capacity (C_p), internal pressure (p_i), free volume (V) of PVC-systems The visco-elastic modules of the composite under volumetric, shear and longitudinal deformation of the material (for φ, T-const and $\omega = 4 \cdot 10^5$ Hz) have also been studied. It has been established that nano-dispersed copper at $0 \leq \varphi \leq 0.60$ vol. %, obtained by the ph/c method, acts as a more active modifier of PVC than EEC. The ways of practical use of PVC-systems in operation in dynamic mechanical and temperature fields are indicated.

Catalytic activity of noble metal nanoparticles deposited over the silica surface in organic pollutants reduction

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In this work the noble metal nanoparticles were deposited over the chemically modified fumed silica surface using method described elsewhere [1]. Fumed silica (A-300) modified with triethoxysilane (TES) (Fig. 1, *a*) was used for noble metals (Pt, Pd, Ru and Au) reduction; for each composite metal loading was of 0.2 mmol/g. The metal reduction reaction and nanoparticles formation were confirmed by FTIR (Fig. 1, *b*) and XRD (Fig. 2), respectively. Size, shape and distribution of nanoparticles on the silica surface were determined from their TEM images.

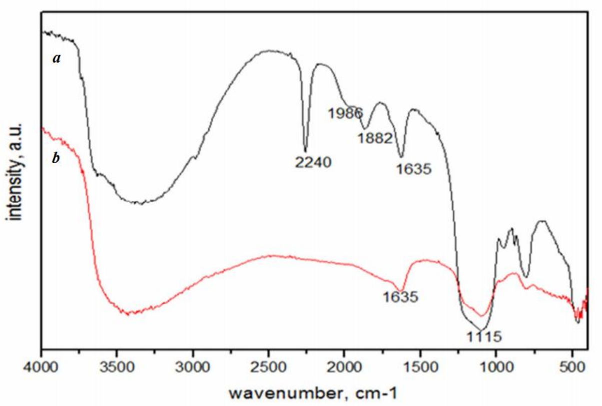

Fig. 1. FTIR spectra of TES-modified SiO_2 (*a*) and after noble metal (Au) deposition (*b*)

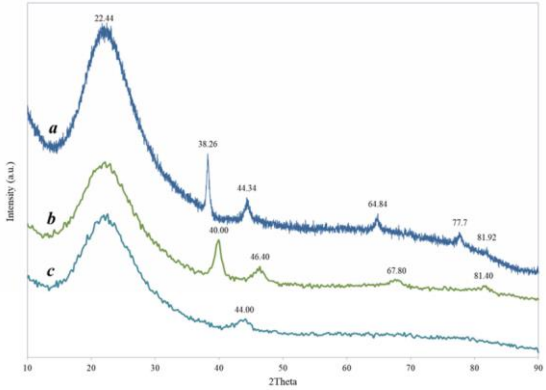

Fig. 2. XRD spectra of gold- (*a*), platinum- (*b*) and ruthenium- (*c*) decorated silicas

All metal-loaded composites were tested in the model reaction of 2-nitrophenol reduction [2] controlled by UV-spectroscopy (TES-modified silica was used as a positive control). It was found that the Pd-decorated silica has a higher efficiency among all tested catalysts, and 2-nitrophenol reduction mechanism corresponds to the pseudo-first-order kinetics. Modified silica without noble metal nanoparticles has no catalytic activity towards the 2-nitrophenol reduction.

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Temperature dependence of a particle flux in a Brownian ratchet with slightly fluctuating potential energy

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Constructing the theory of Brownian motors – diffusion systems creating directed nanoparticle fluxes – allows one to reveal mechanisms and factors that determine characteristics of a motor, and then makes it possible to simulate and design nano-mechanisms possessing desired properties. Depending on the problem being solved, certain approximations are usually chosen, which allow analytical treatment of a problem and obtaining relations for motor characteristics within required ranges of parameters' values.

In previous works, the authors proposed a very promising approximation of slightly fluctuating potential energy [1, 2]: The potential energy is represented as an average relief *u(x)* perturbed by a small fluctuating component *w(x)*. Stochastic fluctuations between the profiles $U_{\pm}(x) = u(x) \pm w(x)$ induce directed particle motion. We continue studying this problem and, adding the Fourier representation within the above approximation, propose a numerical procedure for calculating the particle flux for wide ranges of control parameters.

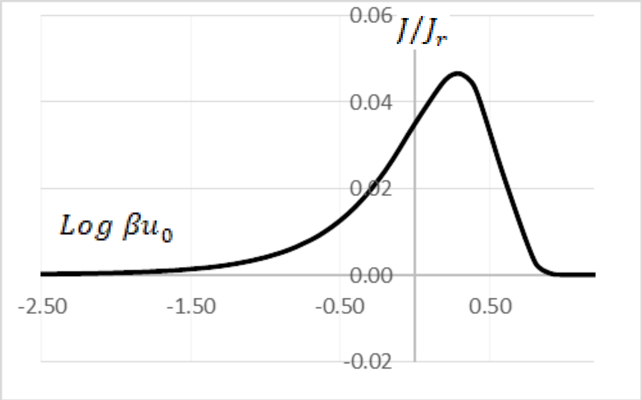

Fig. Temperature dependence of dimensionless flux J/J_r at fixed asymmetry of a sawtooth profile *u*(*x*) and fluctuation frequency

Fig. shows the dependence of the flux *J* on βu_0, $\beta = (k_B T)^{-1}$, for a case of sawtooth *u(x)* [u_0 is the amplitude], and harmonic fluctuating part *w(x)*. The dependence is nonmonotonous, that determines the temperature range of pronounced motor effect and regime in which one can get the largest flux (velocity).

This work has been partially supported by Belarusian Republican Foundation for Fundamental Research (Grant No.Ф18Р-022).

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Li_{1+x}Al surface enrichment: a solution to lithium metal battery

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The high reactivity of lithium and the complex surface structure of the native layer are reasons for fast lithium dendritic growth during the charging process of lithium metal batteries (LMBs). Necessary conditions for the creation of safe and effective lithium electrode are a homogeneity on the Li surface layer and high speed lithium ion diffusion in the volume of solid electrolyte interface (SEI).

Here, it is demonstrated that in the case of the aluminum foil directly contacting lithium on the side of the separator impregnated by electrolyte, the surface superstoichiometric lithium–aluminium alloy (Li_{1+x}Al) is formed *in situ* [1]. The fundamental restructuring of the lithium surface [2, 3] can effectively eliminate the surface inhomogeneity on the lithium surface and increase the ionic conductivity of the SEI. It is observed that a much more uniform lithium dissolution/deposition on the Li_{1+x}Al-modified lithium anode can be achieved as compared to the bare lithium electrode (Fig.).

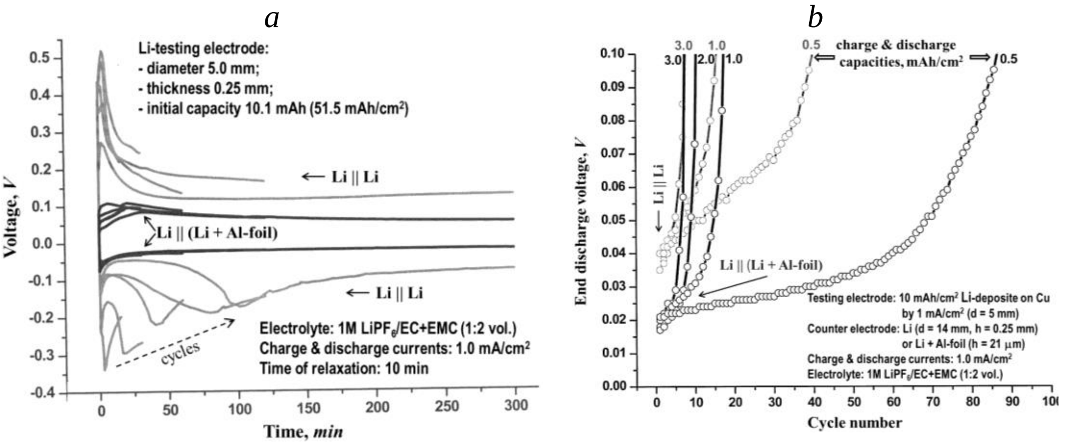

Fig. Electrochemical behavior of Li || Li and Li || (Li+Al-foil) half cells with working electrode prepared from Li-foil (*a*) and via Li-electroplating (*b*)

Compatibility of the Li_{1+x}Al surface enrichment method with mass production process also offers a practical way for enabling Li metal anode for next-generation LMBs.

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TPD MS study of novel materials for solid acid fuel cells

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Fuel cells and electrolyzers are the most efficient devices to convert chemical energy in electrical and vice versa, as they are not limited by thermodynamic efficiency limit (at least not the Carnot's efficiency limit). A major step in bringing fuel cell technology closer to the mainstream market application is developing a solid-state electrolyte system that operates in the intermediate temperature range. The most promising candidate for this system is the solid acid fuel cell (SAFC) [1,2]. Thermochemical studies are very important for the development of new materials for the solid acid fuel cell. Because they allow determining the thermal and long-term stability, the intervals of thermal dehydration, and compatibility of individual components of these multicomponent materials with each other.

In this work, the thermal stability, dehydration processes, decomposition of functional groups of new Pt-based materials for solid acid fuel cells were studied by temperature programmed desorption mass spectrometry (TPD MS). The non-isothermal kinetic parameters of the oxygen desorption, such as the temperature of the maximum desorption rate T_{max}, the reaction order n, the activation energy $E^{\neq}$, the pre-exponential factor ν_0 and activation entropy $dS^{\neq}$, were calculated from TPD MS data [3]. The obtained data for initial sample were: T_{max}=340ºC, n=1, $E^{\neq}$=192 kJ/mol, ν_0=1.26×10^{14} s^{-1}, $dS^{\neq}$=4.7 cal K^{-1} mol^{-1}, R^2=0.967. Kinetic parameters for the sample treated via heating were obtained too: T_{max}=348ºC, n=1, $E^{\neq}$=195 kJ/mol, ν_0=1.70x10^{14} s^{-1}, $dS^{\neq}$=5.1 cal K^{-1} mol^{-1}, R^2=0.953. Treatment shifted T_{max} to a higher temperature and increased $E^{\neq}$ of O_2 desorption. At the same time, the amount of desorbing oxygen decreased by approximately 2-fold for the treated sample, which can be concluded from the comparison of the integrated intensities of the peaks for m/z=32.

Acknowledgements
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Perspective of nanomaterials uses at microbial biotechnology

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Due to the extremely high specific surface of the nanoparticles of different nature and a large surface of microorganisms, they easily enter into contact interaction, as a result of which the cells are largely covered by these particles. Such interaction increases the viability of various types of bacteria, as well as the physiological and biochemical activity of microbial populations.

We have shown that the interaction of different types of bacteria with montmorillonite or palygorskite nanoparticles significantly increases their survival with prolonged storage, as well as at the effects of elevated temperatures. The results obtained are promising for their biotechnological applications. It was established that the addition of 10 g/L of palygorskite nanoparticles to a suspension of *Streptococcus faecium* greatly increased the yield of viable bacteria in the preparation of a dry preparation of these bacteria by spray drying. Such approach was introduced into the production of the drug "Litosil".

It was shown that the growth activity of these microorganisms significantly increased during the cultivation of several types of yeast and bacteria with of silica, aluminoaerosil or clay minerals nanoparticles. The obtained results testify to the promising use of them in the application of investigated strains of bacteria in industrial processes.

The cultivation of nitrogen-fixing and phosphate-mobilizing bacteria with different nanomaterials caused a noticeable effect on the biochemical activity of these microorganisms. On the basis of the interaction of our selected strains nitrogen-fixing bacteria *Azotobacter vinelandii* IMV B-7076 and phosphate-mobilizing bacteria *Bacillus subtilis* IMV B-7023 with bentonite nanoparticles, a granular complex bacterial preparation Azogran was created. It has a stable composition during prolonged storage, improves nitrogenous and phosphorous nutrition of plants, stimulates their growth and development by the biologically active substances of bacterial origin, protects plants against phytopathogens, phytophages and increases their yield crop at 18-37%. Based on the interaction of these bacteria with expanded vermiculite particles, a highly stable form of this preparation has been developed.

The Azogran preparation is registered in Ukraine. For its production, the Institute provided 5 licenses to enterprises of Ukraine, as well as 1 license – to USA firm.

Influence of structure and acid-base characteristics of ZnO on functional properties of Zn-Zr-Si oxide catalysts in ethanol-to-1,3-butadiene process

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Analysis of economic and environmental aspects of realization of ethanol (EtOH) or bioethanol conversion into BD indicates that ethanol-to-butadiene (ETB) process is perspective for industry [1,2]. A rather important problem of the development of catalysts for ETB process lies in the achieving of their high activity and selectivity in the conversion of EtOH-aqueous mixtures [3].

In this study, we have investigated the effect of preparation method of Zn-Zr-Si oxide catalyst on its catalytic properties in the conversion of diluted ethanol mixture into 1,3-butadiene. The zinc oxide and Zn-Zr-Si oxide catalysts were characterized by using several techniques including XPS, XRD, TPD, FTIR and FE-SEM. It is shown that a wet-kneading procedure allows to prepare more active Zn-Zr-Si oxide catalyst comparing to the method of incipient wetness impregnation of the carrier composition with aqueous solution of zinc salt. Also, the use of zinc oxide nanoparticles for the wet-kneading procedure results in more active and selective catalyst compared to the compositions prepared by the same procedure with ZnO macroparticles. The results of investigation of the prepared catalysts by thermo-programed desorption of NH_3/CO_2 and near ambient pressure X-ray photoelectron spectroscopy (NAP-XPS) indicate that the differences in activity could be due to the formation of different acid-base active sites on the zinc oxide surface.

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Physical-chemical properties of the nanocomposites based on magnetite cores and precious metal shells

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The interest in the obtaining of based on ferri- or superparamagnetic cores and precious metal shells nanocomposites is closely connected with their height potential for bio-medical application [1]. Among the traditional synthesis methods we proposed a new one called the rotation-corrosion dispergation (the RCD-method) recently [2]. Green Rust particles phase transformation is spontaneously formed on the iron or steel surface in the open-air system. So, the obtaining of core&shell type nanostructures does not involve the usage of strong chemical reducing agents [3]. Hence, such nanostructures may be applied in the pure biological systems.

The core&shell type nanocomposites formed under the RCD conditions showed X-ray diffraction peaks of magnetite as the core's components, lepidocrocite as a product of Green Rust solid-state oxidation and the reduced precious metal shells. The particle's size varied from 20 to 28 nm depending on the physical-chemical synthesis conditions. The electrokinetic potentials are the following: from (-13.1) to (-24.3) mV for gold-bearing nanoparticles and, correspondingly, from (-13.5) to (-26.7) mV for silver-containing composites. According to X-ray fluorescence spectroscopy the silver fraction in the composites equalled 0.17 and 1.8 mass.% when $c(\mathrm{Ag}^+)$ reached 1 and 20 $\mathrm{mg \cdot dm^{-3}}$, respectively. Whereas the gold fraction in the composites in both cases was smaller comprising 0.05 and 0.9 mass.% at the Au^{3+} concentrations 1 and 20 $\mathrm{mg \cdot dm^{-3}}$. Magnetic study of core&shell type nanocomposites showed their super paramagnetic properties when the saturation magnetisation of the samples was varied from 24 to 48 $\mathrm{A \cdot m^2 \cdot kg^{-1}}$.

In addition, the gold-contained nanocomposites showed distinctive optical properties. Under broadband light source 500-650 nm, they demonstrated shift of the plasmonic peak to far red frequency range that is corresponded to 'transparency window' for body tissues. So, core-shell nanocomposite $\mathrm{FeFe_2O_4\&Au^0}$ have a good prospects for biomedical applications, especially as the molecular therapeutics platform.

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On the chemical nature and efficiency of nitrogen species' incorporation in titania lattice obtained by PLD procedure

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Nitrogen-doped titania has been considered as a perspective material for ecological photocatalysis. The presence of nitrogen in semiconductive lattice leads to the change of the electronic structure of titania, surface morphology and crystallinity degree. Despite of numerous scientific reports concerned its properties, there are still a number of key questions connected to the role of nitrogen species. Among them, the chemical nature and location in the solid because these parameters can strongly influence the surface reactivity and photocatalytic properties of the materials.

Nitrogen-doped titania films obtained by pulse laser deposition method (PLD) using titanium foil as a target in N_2:CH_4=5:1 atmosphere at different gas pressures (3, 10 and 100 Pa) and treated at 450 °C have been investigated by XPS, SEM and EDS techniques to clarify the degree of nitrogen incorporation and the nature of incorporated species, the ratio of the elements on the surface and bulk as well as the morphology of surface.

As shown by XPS, the content of incorporated nitrogen on the surface is decreased in 4 times with increasing the gas pressure from 3 to 100 Pa in the system. It points on the influence of N_2 and CH_4 contents on the efficiency of N incorporation. The detailed deconvoluted XPS spectra of N1*s* region revealed that nitrogen is incorporated in different chemical states, as namely substitutional, interstitial and other N species. As one more evidence of such species formation, the XPS spectra of Ti2$p_{3/2}$ peak contain three maxima belong to Ti-Ti, Ti-N and Ti-O bonds. Additionally, the formation of such bonds can be also confirmed by split spin-orbit components of Ti2*p* peaks.

The oxygen atoms' content in the bulk is significantly increased for the film obtained at 100 Pa in comparison with the other ones. Thus, comparing the ratio Ti to O obtained in the bulk (EDS) and on the surface (XPS), one can be noted that the less nitrogen on the surface is detected, the more oxygen is present on the surface as well as in the bulk of the materials.

Morphology of surface is also changed depending on the gas pressure as shown by SEM images: the PLD procedures at 3 and 10 Pa lead to formation of non-porous structure while well-ordered porous layer is observed at 100 Pa.

Sorption of natural flavonoids on the nano alumina surface

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Flavonoids supplied to human organisms with food can be a source of natural antioxidants, among them quercetin and rutin are the most often isolated and analyzed. These compounds are part of medicinal plants, food products, dietary supplements, and are widely used in medicine due to various pharmacological activities. The purpose of this work was to determine the patterns of natural flavonoid sorption on the nano alumina surface in dependence on concentration and pH of their water-ethanol solutions to develop the assays of the sorption-spectrophotometric determination of quercetin and rutin in preparations of plant origin.

Complex sorption and spectral studies of the interaction of rutin and its aglycone quercetin with highly dispersed aluminum oxide were carried out. The flavonoid sorption starts at pH>2.5 and becomes maximal in the neutral medium, correlating with the content of non-dissociated surface ≡AlOH groups. Both quercetin and rutin sorption is described with the type-H isotherm which is typical for the chemosorption. The found coincidence of spectral characteristics of flavonoids on the alumina surface and in solutions containing Al(III) ions indicates the formation of similar chelate complexes in these systems.

It was found that the spectral characteristics (intensity and position of the absorption bands) of flavonoids sorbed on the surface of aluminum oxide depend on their concentration and pH of aqueous solutions. The intensity of sorbent colour is proportional to the surface concentration of quercetin and rutin and values of their conditional molar absorption coefficients in 0.025% alumina dispersion (ε^{S}_{434}= 4386 g/mole·cm and ε^{S}_{403}= 5280 g/mole·cm respectively) were determined. In addition, the absorbance of dispersion (A_{disp}) linearly depends on the concentration of quercetin and rutin in analyzed solutions and is described by the equations of the calibration curves given in the Table.

Table. Calibration equations in coordinates "A_{disp} – the concentration of quercetin (C_{Querc}) and rutin (C_{Rutin}) "

Flavonoid	$\lambda_{\max}$, nm	Equations of the calibration curves	*R*
Quercetin	434	$A_{\mathrm{disp}}=(0.001\pm0.003)+(1.216\pm0.036)\cdot 10^4\cdot C_{\mathrm{Querc}}$	0.998
Rutin	403	$A_{\mathrm{disp}}=(0.004\pm0.004)+(1.613\pm0.058)\cdot 10^4\cdot C_{\mathrm{Rutin}}$	0.997

Thus, nano alumina is found to be a promising solid-phase reagent for the determination of quercetin and rutin in preparations of medicinal plants by spectrophotometric or visual test methods.

Electrophysical properties of FeCo and carbon nanotubes/FeCo composites

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To date, a lot of nanostructural metallic composite materials on the basis of carbon nanotubes have been synthesized for obtaining electromagnetic and gas sensor devices, catalysis, antifriction coatings, and others.

The purpose of this work is to synthesize composites of FeCo and multilayer nanotubes/FeCo (MWNT/FeCo) and to establish differences in their electrophysical properties, depending on the nature of the surface.

Two consignments of MWNT/FeCo composites were synthesized using conventional MWNT. Synthesis was carried out by the method of co-precipitation from a solution of hydrazine hydrate of salts iron, cobalt and aqueous suspension of nanotubes (was pre-treated with ultrasonic dispersant).

The composite materials were investigated using an electron microscope, X-ray diffraction and electrophysical methods in the high and low frequencies. Investigation of the real (ε') and the imaginary (ε") components of the complex dielectric permittivity of composites was made in ultra-high frequency (UHF) ranging 8-12 GHz and using an interferometer RFK-18 which was based on measuring of the phase difference, standing wave ratio and the weakening of R2-60 by the no-electrode method. And the conductivity was made at low frequencies of 0.1, 1 and 10 kHz were made with two-contact method using immittance meter E7-14. The results are presented in the Table.

Table. Electrophysical characteristics of FeCo and MWNT/FeCo composites

	Complex permittivity in the range of 8-12 GHz		Magnetic permittivity on frequency 8 GHz		Conductivity σ on 1kHz, $Om^{-1}cm^{-1}$
	ε′	ε″	μ'	μ″	
FeCo	5.6	4.2	1.55	0.15	0.26
MWNT/FeCo	2.3	0.58	1.17	0.025	$6.3\cdot10^{-6}$

The low frequency conductivity and electrophysical parameters in the microwave range of FeCo composites are higher than MWNT/FeCo due to the greater concentration of the metal component.

The composites effectively interact with electromagnetic radiation, the technology used allows the controlled change in the properties of composites within specified limits.

Activation of aluminum by doping with low-melting metals and regularities of its hydrolysis

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The hydrolysis of aluminum is a promising way of hydrogen generation directly at the point of use. Aluminum has a high negative value of standard electrode potential and reacts with water easily and quickly when the passive oxide layer on its surface is absent. Different methods can be applied for aluminum activation: mechanical, mechanochemical, chemical, *etc*.

In the present work aluminum was doped with low-melting metals (Ga, In, Sn). Previously prepared eutectic alloy Ga-In-Sn (67/22/11 wt.%) was liquid at room temperature (melting point 10.7 ± 0.3 °C). Aluminum based alloys were fabricated in an electric furnace (900 °C, 30 min) under argon with mechanical mixing. The regularities of the hydrolysis of prepared Al based alloys were studied by volumetric measurements of evolved hydrogen at regular intervals. Samples of alloys with a mass of 1 g were immersed into 100 ml of distilled water at 25 °C. After bringing evolved hydrogen volumes to normal conditions, plots of hydrogen volume as well as the rates of hydrogen accumulation and evolution *vs* hydrolysis duration were obtained (see Fig.).

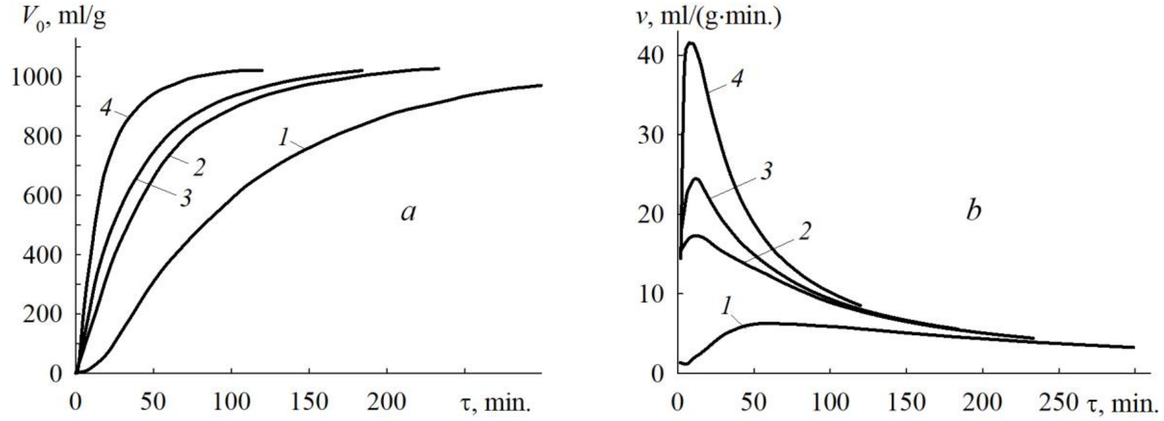

Fig. Plots of hydrogen volume (*a*) and the rate of its accumulation (*b*) *vs* duration of hydrolysis of aluminum alloys with mass fractions of eutectic Ga-In-Sn (%): (*1*) 3, (*2*) 5, (*3*) 7, (*4*) 10

All investigated Al based alloys reacted with water at 25 °C and cracked into small pieces. The rates of hydrogen evolution significantly increased when the percentage of Ga-In-Sn alloy in aluminum alloys was raised from 3 to 10 %. The hydrolysis of thus activated aluminum proceeded practically to the end, and hydrogen yield was close to 100 %.

Nano-bio interactions: adsorption of the nucleotides onto nanocrystalline titania surface

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With the advance of nanotechnology, a vast diversity of nanomaterials has been developed for a wide range of applications. In the context of their biomedical applications and toxicity, these nanomaterials are exposed to various biomolecules. The investigation of the interaction between these molecules and nanoparticles is quite difficult. One of the approaches to solve this problem is the way of model studies of the interaction of individual biomolecules with nanooxide surfaces. The aim of this work is the investigation of adsorption of adenine nucleotides with different length of phosphate chain at the titania/aqueous solution interface in terms of surface complexation theory. Adsorption of adenosine-5′-mono-, di-, and triphosphates (AMP, ADP, and ATP) on the surface of nanocrystalline anatase (pzc=6.5) was studied as a function of pH and ionic strength of solution (Fig.).

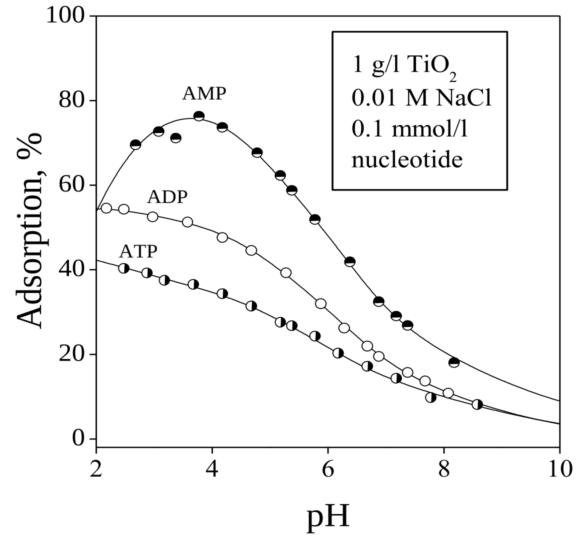

Fig. The adsorption of nucleotides as a function of pH

The obtained results were used to calculate the equilibrium reaction constants on the TiO_2 surface (Basic Stern model, GRFIT program). In order to select possible complex formation reactions it is necessary to take into account the state of the surface groups of solid and the forms in which nucleotides are present in solution depending on pH. It was suggested that the nucleotide complexes are formed due to the electrostatic interaction of nucleotide anionic forms with protonated surface groups $TiOH_2^+$.

Nucleotide surface complexes with different phosphate chain lengths contain anions that vary in charges. The nature of the interaction between anions and surface groups is confirmed with the results of the nucleotide desorption study by the equilibrium dialysis method.

Electrophysical characteristics of polymer nanocomposites based on calcium ferrite modified with copper iodide

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Nanomaterials have attracted much attention as novel electromagnetic wave absorbers due to their small size and high surface energy. Research mainly focuses on nanoferrite, metal nanoparticles, nanofibers *etc*. Nanoferrites offer the unique potential to be excellent absorption materials due to their low cost, high absorption efficiency in the wide frequency band.

To create such materials, nanocomposites based on calcium ferrite have been synthesized. $CaFe_2O_4$ was synthesized using the modified sol-gel technique. The prepared powder was ground and the heat treatment was carried out at 1123 K for 5 hours. The samples $CaFe_2O_4$ were prepared by a chemical method during the course of release of CuI from an aqueous solution in the presence of $CaFe_2O_4$. The samples of system $CuI/CaFe_2O_4$–polychlorotrifluoroethylene (PCTFE) was compacted at the temperature equal to the melting point of the polymer at a pressure of 2 MPa. Original calcium ferrite and composites $CuI/CaFe_2O_4$ were investigated by X-ray analysis (XRD). The real (ε') and imaginary (ε'') components of the complex permittivity in microwave range were measured using the interferometer at a frequency of 9 GHz. The real (σ') and imaginary (σ'') components of the complex electrical conductivity ($\sigma^*=\sigma'+i\sigma''$) at low frequencies (0.1, 1 and 10 kHz) were measured using the immittance meter E7-14 by two-contacts method at 295 K.

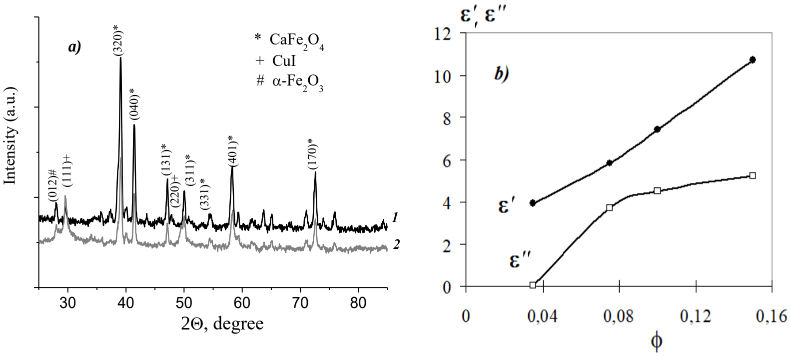

Fig. X-ray diffraction patterns of synthesized nanoparticles: *1* – $CaFe_2O_4$, *2* – $0.32CuI/CaFe_2O_4$ (*a*), dependence of ε' and ε'' at a frequency of 9 GHz polymer nanocomposites on volume content (ϕ) of copper iodide in systems $0.32CuI/CaFe_2O_4$–PCTFE (*b*)

Our identification of the observed diffraction XRD maxima provides evidence for the fact that in the samples $CuI/CaFe_2O_4$ copper iodide is in cubic modification (Fig., *a*). Surface modification of ferrite with CuI leads to a significant increase in the values of ε', ε'' and σ of both the low and high frequencies (Fig., *b*).

Controllable design of aminosilica microparticles for multi-uses

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During the past decade, silica particles with amino groups have been broadly investigated [1-3] and now they are a commercial product of various chemical companies, including Sigma Aldrich. Their application for solving many practical problems, including such global as ecological, energy-saving and medical, has attracted attention of scientists to their synthesis and study. Also, aminosilica particles are important due to their economic efficiency and eco-friendliness. We optimized the reaction conditions between silica structuring agent and 3-aminopropyltriethoxysilane leading to the control of the main characteristics of the particles such as size, porosity, amino groups content and availability, zeta potential. It could be achieved by introduction of alkyl-containing silanes, adjustment of reagents ratio, temperature, reaction timing and catalyst. Besides, as advanced nanomaterial, bifunctional nanoparticles exhibit special properties because they integrate the benefits of two types of ligands, amino group and organic group. Such bifunctional microparticles manifested excellent performance when applied in metal ions [4-5] or dyes adsorption [6], antibacterial activity assay [5,6]. Overall, further elaboration of this research direction is a challenging task.

Acknowledgements
I.V. Melnyk and M. Vaclavikova are grateful for the financial support from the project VEGA 2/0156/19.

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MXene sorbents for removal of urea from dialysate – a step towards the wearable artificial kidney

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The wearable artificial kidney can deliver continuous ambulatory dialysis for more than 3 million patients with end-stage renal disease. However, the efficient removal of urea is a key challenge in miniaturizing the device and making it light and small enough for practical use. Here we show that two-dimensional titanium carbide (MXene) with the composition of $Ti_3C_2T_x$, where T_x represents surface termination groups such as –OH, –O–, and –F, can adsorb urea, reaching 99% removal efficiency from aqueous solution and 94% from dialysate at the initial urea concentration of 30 mg/dL, with the maximum urea adsorption capacity of 10.4 mg/g at room temperature. The comparison of various MXenes showed that $Ti_3C_2T_x$ had higher adsorption capacity than Ti_2CT_x and $Mo_2TiC_2T_x$ in both aqueous solutions and dialysate. When tested at 37°C, we achieved a twofold increase in the urea removal efficiency from dialysate by $Ti_3C_2T_x$, with the maximum urea adsorption capacity of 21.7 mg/g. The fact that the urea removal efficiency from dialysate is comparable with the efficiency of removing urea from aqueous solution in the absence of competing adsorbates suggests that $Ti_3C_2T_x$ shows selectivity towards urea adsorption, probably owing to narrow slit pores between negatively charged MXene sheets that allow selective adsorption. $Ti_3C_2T_x$ showed good hemocompatibility; it did not induce cell apoptosis or reduce metabolising cell fraction indicating no impact on cell viability at concentrations of up to 200 μg/mL. Healthy donor haemocompatibility assays indicated no impact on blood clotting, haemolysis and platelet activation following 60-min incubation indicating MXenes are safe to use for blood contacting applications. The biocompatibility of $Ti_3C_2T_x$ and its selectivity for urea adsorption from dialysate open a new opportunity in designing a miniaturised dialysate regeneration system for a wearable artificial kidney. To the best of our knowledge, this is the first report of a physical adsorbent which has such selectivity and adsorption capacity towards urea.

Morphology and mechanical properties of metal-filled composite based on immiscible polymer blend

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Polymer composites based on immiscible polymers blend are a new type of structural materials with designed morphology. Such composites can significantly change their properties depending on the ratio of polymer phases in the composite.

The composite studied (PP/CPA-Fe) was prepared in two stages, at first co-polyamide (CPA) was extruded with 40 % vol. of Fe particles (average size is 2-3 μm), then this concentrate was diluted by the pure polypropylene (PP) using extrusion as well. Samples were produced by hot pressing from the extrudate in a form of disks with a diameter of 30 mm and a thickness ~ 2 mm.

Morphological study of the composites was carried out using optical microscopy and showed that Fe particles are localized only in the CPA phase. Three different regions can be distinguished in the whole concentration range of PP/CPA-Fe composite: 1) in the region from 0 to 7% vol. the CPA-Fe phase is distributed in a form of separate inclusions and PP is the composite matrix; 2) from 7 to 16% vol. there is the region where phases CPA-Fe and PP are co-continuous and create the region of phase inversion; 3) in the region from 16 to 30 % vol. phase CPA-Fe becomes as a matrix in the composite, while PP creates the separate inclusions.

Investigated thermomechanical characteristics correspond to the morphology of composite. Relative deformation (ε) and storage modulus (G') of the composite demonstrate three families of curves that reflects the structural features of a composite.

At low filler concentration, the main thermomechanical properties of PP/CPA-Fe are defined by its PP matrix. The region of phase inversion is characterized by two inflection points corresponding to each polymer component in the co-continuous structure. At high filler content the main contribution to the thermomechanical properties of the composite gives the CPA-Fe phase.

Thus, by changing the phases ratio in the composite based on immiscible polymers blend, it is possible to achieve a significant change in its properties, in particular, mechanical ones.

Formation of gold nanoparticles in $HAuCl_4$ / Na citrate system depending on concentration of components, temperature and pH

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The application areas of gold nanoparticles (Au NPs) are expanding firmly taking place among chemical and biological sensing, biomolecular imaging, diagnostics and therapy. Commonly, for the preparation of nanosized gold for biological use the "citrate" method is used. At the same time this classical procedure should be revised as minor changes in experimental parameters greatly affect the whole colloidal system. Specifically, the mechanism of particles formation and their interaction causes aggregation that further appears as a loss of stability of colloids during storage.

Dynamic light scattering (DLS) method is suitable for the investigation of size distribution of nanoparticles in Au NPs colloid and their aggregation state. Comparative analyses of UV-vis spectra with DLS data by number, volume and intensity basis allow us to trace the changes in Au NPs colloid in time.

We performed UV-vis and DLS analyses on series of citrate-stabilized Au NPs, obtained with different experimental procedures varying 1) the ratio of reagents, 2) their concentrations, 3) the initiation temperature of reaction and 4) the duration of heating, 5) the order of introduction of reagents into the reaction mixture, 6) pH and so on.

Usually the position of the maximum of localized surface plasmon resonance (LSPR) band of gold in absorption spectra is associated with the size of Au NPs, while band's width and symmetry contain information about aggregation processes. We find the correlation between LSPR band position and shape with DLS data obtained by intensity basis. At the same time size distribution by number and volume reflected the completeness of the process of particle formation accompanied with continuous growth due to ripening processes.

Optimal conditions were found to produce Au NPs with prolonged stability ensured by negatively charged citrate shell around particles. Thus, by varying approaches and parameters of the reaction, we can achieve tailored properties of nanosized gold.

Design, synthesis and biological properties of C_{60}-lactate complexes

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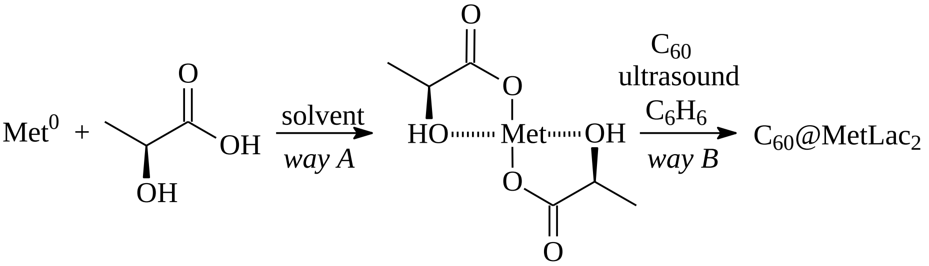
As you know, fullerene has unique physical, chemical and biological properties. Synthesis of new fullerene derivatives opens wide opportunities for their use as new drugs. On the other hand, such biological molecules as metal lactate have the ability to coordinate on the spherical aromatic surface of fullerene and form stable C_{60}-lactate complexes. Thus, we can obtain substances with new biological properties and use them as, for example, promising muscle relaxants during of the trauma therapeutically period.

Within this framework, we suggest using Mg^{2+}, Ca^{2+}, Sr^{2+}, Zn^{2+} as a strong complexing agents, with lactic acid anion and fullerenes C_{60} as ligands.

We have performed a quantum-chemical analysis of possible complexing of $MetLac_2$ (Met = Mg^{2+}, Ca^{2+}, Sr^{2+}, Zn^{2+}) with fullerene C_{60}, using MM+, PM3 and Monte-Carlo methods. There has been calculated the optimal structures, absorption spectra of C_{60} with various amounts of $MetLac_2$ on the spherical surface of the latter. There has been found a constant of complex's stability which is 68.5 $l \cdot mol^{-1}$ (for the $MgLac_2$); 55.3 mol^{-1} (for the $CaLac_2$); 98.5 $l \cdot mol^{-1}$ (for the $SrLac_2$); 108.2 $l \cdot mol^{-1}$ (for the $ZnLac_2$) in accordance ($k_{korr} \geq 0.98$).

A series of *d*-block metal lactates was obtained *via* "direct synthesis" strategy based on the use of metals/oxides as the starting materials (*way A*):



where Met^0 = Mg, Ca, Sr, Zn; Solvent = CH_3OH, DMF, DMSO, H_2O.

A two-phase system consisting of an aqueous solution of lactate and a solution of fullerene in benzene was treated an ultrasound (frequency = 22 kHz, intensity = 50 W/cm^2, time = 1 min), see *way B*. Composition and structure of the compounds were characterized by means of elemental analyses, UV-Vis, IR spectroscopy, ^{13}C-NMR.

The thesometric studies on the calcareous and cambaloid medial muscles of rats have been carried out to detect the influence of the obtaining complexes.

Silver nanoparticles photogeneration in cross-linked Dextran-graft-Polyacrylamide hydrogels

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Hydrogels are crosslinked 3D networks of hydrophilic polymer chains, are capable of holding large amounts of water. Since water is the greatest component of the human body, a hydrogel, which can absorb large quantities of water, is considered to have great potential when applied for biomedical purposes. Recently, wide investigation has been going on into the feasibility of applying hydrogels in fields including tissue engineering, drug delivery, self-healing materials, biosensors, hemostasis bandages and wound dressing.

In the treatment of chronic wounds the principal aims are typically to prevent infection while allowing the wound to heal. This study therefore sought to prepare the hydrogel pads based Dextran-graft-Polyacrylamide with incorporated silver nanoparticles (AgNPs). We varied the molecular weight of Dextran component during hydrogel synthesis, the hydrolysis degree of polymer hydrogel, concentrations of $AgNO_3$ as well as irradiation time for reduction of Ag^+ into AgNPs.

We used UV light irradiation for reducing of silver precursor $AgNO_3$ into crosslinked polymer matrix. Hydrogels with incorporated AgNPs were studied by UV–vis absorption, Scanning Electron Microscopy and FTIR.

It is shown that the increase of irradiation time accompanies by the absorbance intensities increase of AgNPs, meanwhile, the maximum of absorption peak demonstrates a slight red-shift to 435 nm that can be explained by the growing in sizes and quantity of AgNPs. At the same time, the nanoparticles diameters and distribution range depend on the concentration of anionic groups in hydrogels obtained at different hydrolysis time of cross-linked Dextran-graft-Polyacrylamide copolymer. SEM-studies of surface morphology confirmed that chemical nature of hydrogel (non-ionic or anionic) doesn’t affect drastically the size of AgNPs synthesized *in situ*. The FTIR spectra of the hydrogel and hydrogel/AgNPs nanosystems point on some differences indicating weak interaction between $-NH_2$ groups of polymer chains and AgNPs as well as stabilization of nanosystem.

Results of microbiological investigations of Dextran-graft-Polyacrylamide with incorporated silver nanoparticles confirm that they can be used for biomedical applications as wound of various genesis dressing, artificial burn dressings and tissue technology.

DFT study of hydrogen interaction with sulfur moieties in natural graphite

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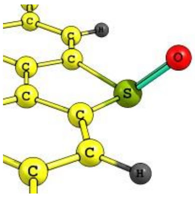
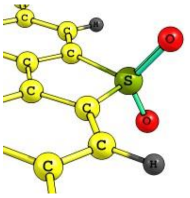
The natural graphite flakes contain a detectable amount of sulfur impurities in the form of heterocyclic bound sulfur [1] and require further purification for application in the functional materials. The aim of the present study was the quantum chemical simulation of hydrogen interaction with sulfur moieties in natural graphite.

The process of interaction of hydrogen with sulfur atom was simulated using the density functional theory method. All calculations were carried out using the B3LYP exchange-correlation functional and valence-split basis set expanded with polarization functions (3-21G**).

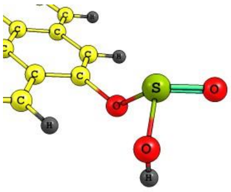
The considered models contain sulfur atom embedded in the graphite network (*a*, *b*) and as a functional group (*c*, *d*, *e*).



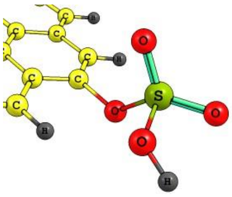
sulfoxide (*a*)



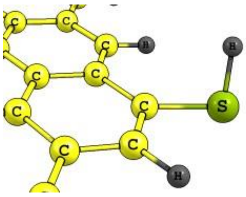
sulfone (*b*)



sulfite (*c*)

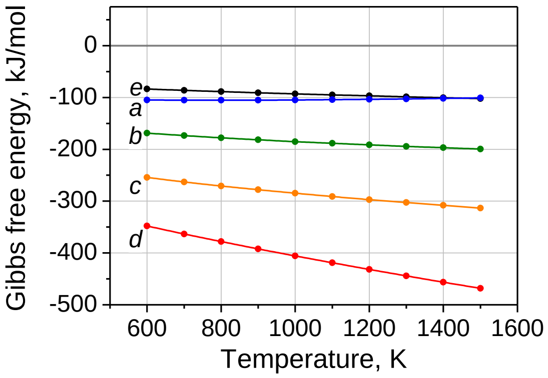


sulfate (*d*)



thiol (*e*)

The Gibbs free energy (ΔG) for the considered sulfur moieties and corresponding reactions were calculated within 600–1500 K temperature interval.



(*a*) $C_{40}H_{14}SO + H_2 = C_{40}H_{14}O + H_2S$

(*b*) $C_{40}H_{14}SO_2 + 2H_2 = C_{40}H_{14}O + H_2S + H_2O$

(*c*) $C_{42}H_{15}–OS(O)OH + 3H_2 = C_{42}H_{15}–OH + H_2S + 2H_2O$

(*d*) $C_{42}H_{15}–OS(O)_2OH + 4H_2 = C_{42}H_{15}–OH + H_2S + 3H_2O$

(*e*) $C_{42}H_{15}–SH + H_2 = C_{42}H_{16} + H_2S$

Fig. Temperature dependences of the Gibbs free energy for the reactions of hydrogen with sulfur moieties

The reactions between hydrogen and sulfur moieties (Fig.) appear to be thermodynamically favourable within the entire temperature interval.

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Combined FT-IR spectroscopic and mass-spectrometric studies of cinnamic acids on the surfaces of alumina and nanoceria for biomass conversion

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Recently, more and more attention has been paid to the conversion of biomass, in particular lignocellulose, as a renewable raw material, in order to obtain a number of valuable bio-based chemicals. One of the important tasks in developing new environmentally friendly technologies of heterogeneous pyrolysis of biomass is the search for selective catalysts, the application of which will allow to varying the final products of transformations of biomass components, their final output and optimal temperatures of these processes.

Pyrolytic methods are powerful instruments for using in the field of conversion of renewable biomass components [1,2]. In this work, a comparative study of the thermal transformations of caffeic acid (CA), ferulic acid (FA) and chlorogenic acid (ChA) on the CeO_2 and Al_2O_3 surfaces was performed using the method of temperature-programmed desorption mass spectrometry (TPD MS) in conjunction with the Fourier transform infrared spectroscopic analysis. CA, FA and ChA are structural units of lignocellulose biomass. It was found that the interactions of CA and FA with the surfaces of alumina and nanoceria occur through both carboxyl and phenolic functional groups. The pyrolysis of these complexes is accompanied by intense decarboxylation and decarbonylation processes. The formation of compounds of 3,4-dihydroxy-phenylethylene (*m/z* 136, 110–550 °C), pyrocatechol (*m/z* 110, $T_{max} \approx 260$ °C) and hydroxybenzene (*m/z* 94, $T_{max} \approx 390$ °C) takes place during pyrolysis as a result of the transformation of CA complexes on CeO_2. In contrast the CA complexes on Al_2O_3 are preferably decomposed with the formation of low molecular weight phenol products: hydroxybenzene (*m/z* 94, $T_{max} \approx 408$ °C) and cresol (*m/z* 108, $T_{max} \approx 376$ °C).

Acknowledgements
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TPD-MS study of a surface layer of fumed silica modified by polydimethylsiloxane

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Hydrophobized fumed silica has a practical potential for using as a filler of nonpolar or weakly polar polymers. The physicochemical properties and characteristics of the modified composites depend on the concentration, structure of grafted functional groups or polymers (e.g., $Si(OR)(CH_3)_2$, $Si(CH_3)_3$, depolymerized polydimethylsiloxane (PDMS) molecules), as well the degree of substitution of surface silanols. The temperature-programmed desorption method with a mass-spectrometry (TPD-MS) control allows one to distinguish surface hydroxyl structures of various types including adsorbed water on fumed silica surface modified with PDMS. A TPD-MS study of water (*m/z* 18), CO (28) and CO_2 (44) desorption (under heating up to 1000 K) from a surface of silica modified by PDMS of various molecular weight (M_w) in the presence of dimethyl carbonate (DMC) as a catalyst was carried out. The desorption of molecularly adsorbed water is observed at 350-450 K, and desorption of associatively desorbed water occurs in the range of 500-900 K (Fig.). An increase in the intensity of the peaks of water, CO, and CO_2 desorption is observed with changing both in the concentration and M_w value of PDMS. The strong interactions of attached and adsorbed polymers with the silica surface cause changes in the mechanism of the thermal decomposition of the surface functional layer.

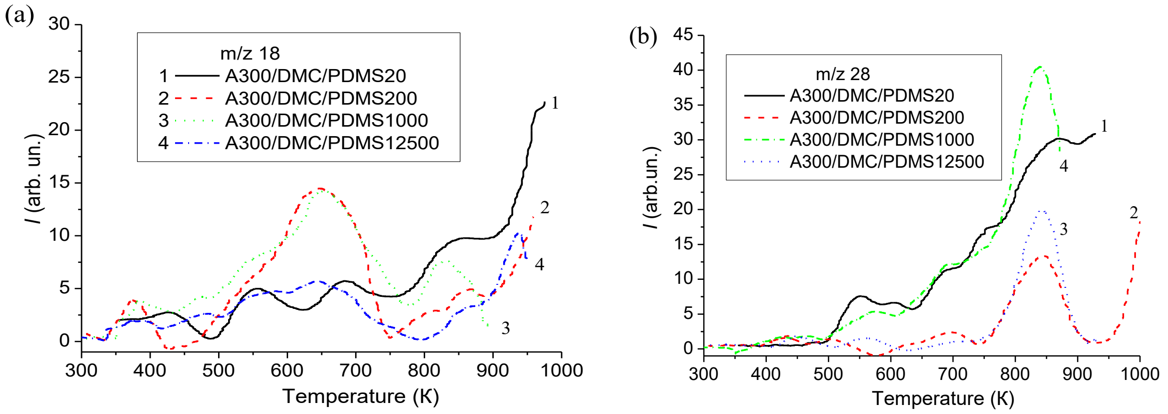

Fig. TPD-MS spectra of (*a*) water (*m/z* 18) and (*b*) CO (*m/z* 28) desorption from composites

Influence of acid treatment on the structural properties of lignocellulosic complex of apricot seed shells

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Fruit seed shells refer to annually renewable raw material, which is a complex of organic polymers with valuable properties, including sorption ones. In crude form, such materials are characterized by low sorption properties. The absorption characteristics of plant materials depend on their chemical composition and structure which can be improved with the application of mechanical (grinding), chemical (hydrolysis or delignification) and physical (hydrothermal) treatments.

The purpose of the work is to study the influence of acid treatment conditions on structural properties of lignocellulosic complex from apricot seed shells. The treatments of initial material with mineral and organic acid on the first stage were carried out at 102°C during 1 h, and the acid concentrations were 4 and 7.5%, respectively. The second stage involved alkaline treatment of plant materials with alkali solution. The chemical composition of obtained materials and their surface areas are given in Table.

Table. Sorbents composition and surface area characterization

Samples	Chemical composition			Surface area (BET), m^2/g
	Lignin,%	Cellulose, %	Ash, %	
Initial apricot seed shells	63.15	42.53	2.6	3.5
Apricot stones modified with HCl	61.74	26.93	1.5	4.5
Apricot stones modified with $C_6H_8O_7$	52.17	46.02	0.3	2.1

As can be seen, application of HCl leads to depolymerization and degradation of polysaccharide components as the cellulose content is reduced. The treatment of shells with organic acid results in obtaining sorbent with lower surface area due to partial delignification as the lignin content is decreased. Both treatments allow to reduce ash content in final materials.

The obtained results indicate the feasibility of mineral acid modification of apricot seed shells to increase the porosity of the lignocellulosic materials.

Sorption of lead(II) ions by plant sorbents based on lignocellulose and pectin

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The pharmaceutical market is annually replenished with new sorption products based on plant polymers: pectin, lignin and cellulose. Many scientific papers, which consider sorption of heavy metals by plant enterosorbents, have currently been developed. However, very little attention is paid to the sorption of lead(II) ions, which belongs to the group of the most dangerous ecotoxicants (carcinogens), can accumulate in the human body and, consequently, has a lasting poisonous effect.

The purpose of this work is to study the sorption capacity in relation to lead ions of Dietary supplement "Celisorb" (TU U 10.8-03291669-010: 2018), Dietary supplement "Pectin complex" (TU U 15.8-16475490-001: 2001), as well as a number of lignin- and pectin-containing materials.

Sorption experiments (Fig.) have carried out in static conditions using ($Pb(CH_3COO)_2{\cdot}H_2O$) saline solutions with different concentrations, at different pH levels and on a standard salt solution (Ringer's solution).

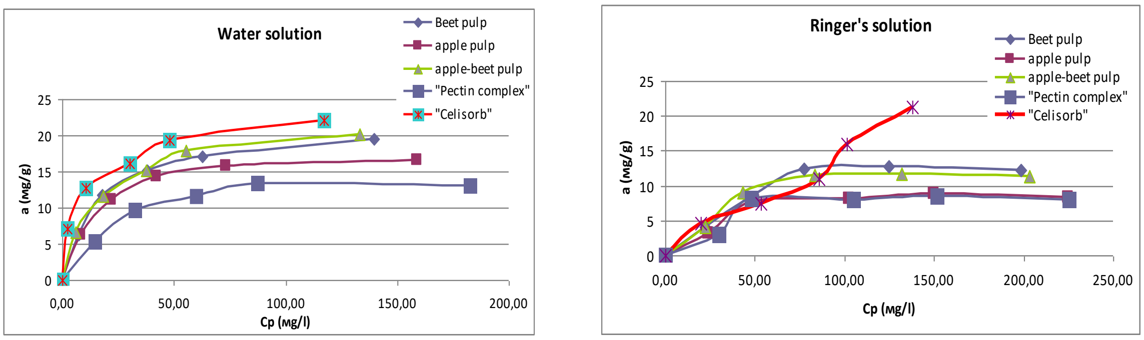

Fig. The isotherms of sorption of lead(II) ions by lignin- and pectin-containing materials from aqueous medium and from a Ringer's solution

The obtained quantitative characteristics of the sorption of heavy metal ions by enterosorbents of different origin and pectin-containing materials make it possible to purposefully use them as dietary supplements and medical preparations, aimed at removal of a lead from an organism.

Reagents and methods for cloud seeding

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Weather modification reduces the negative effects of climate change and damage from natural disasters. Currently, the main way to control the weather is chemical influence on hydrometeorological processes. It is carried out with the help of special substances that cause the formation of ice particles in the clouds - ice-forming reagents.

An analysis of the weather modification was made. Based on it, it was concluded that currently used ice-forming reagents and methods for their dispersion have reached their limit. Progress in this area is possible primarily creating new, more efficient reagents - powdery nanoscale reagents based on the levelity principle.

In the 80s at the Chuiko Institute of Surface Chemistry (CISC) the highly disperse nanoscale silica (nanosilica) was chosen as an inert carrier. Inorganic and organic substances with ice-forming activity were applied onto the nanosilica surface nanoparticles by adsorption modification. However, technical problems did not allow to turn a laboratory method of obtaining a new type of crystallizing reagents into real technology.

In recent years, CISC has developed methods for gas-phase solvate-stimulated modification of nanosilica with inorganic salts and non-volatile organic compounds at the atmospheric pressure. This made it possible to simplify significantly the process of formation of a layer or clusters of ice-forming substances on the nanoparticles surface and make it as technologically advanced as possible.

Several nanoscale ice-forming AgI/SiO_2 reagents were synthesized using new technologies. The tests of the ice-forming activity of these samples showed their effectiveness.

Acknowledgements

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Polyvinylidene fluoride membranes modified with TiO_2 nanoparticles for beer filtration

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Membrane modifying with nanoparticles with photocatalytic properties is a promising method to prevent fouling of membrane surface. For this purpose, TiO_2, ZnO, SnO_2 nanoparticles and their composites are widely used.

Polyvinylidene fluoride membranes with cut-off of 150 kDa were modified with polyetheleneimine (PEI) and TiO_2 nanoparticles. Unfiltered beer “Opillia” was used to evaluate membrane fouling in the dead-end mode. Dependence of the volumetric flux on an applied pressure for membranes is presented in Fig.

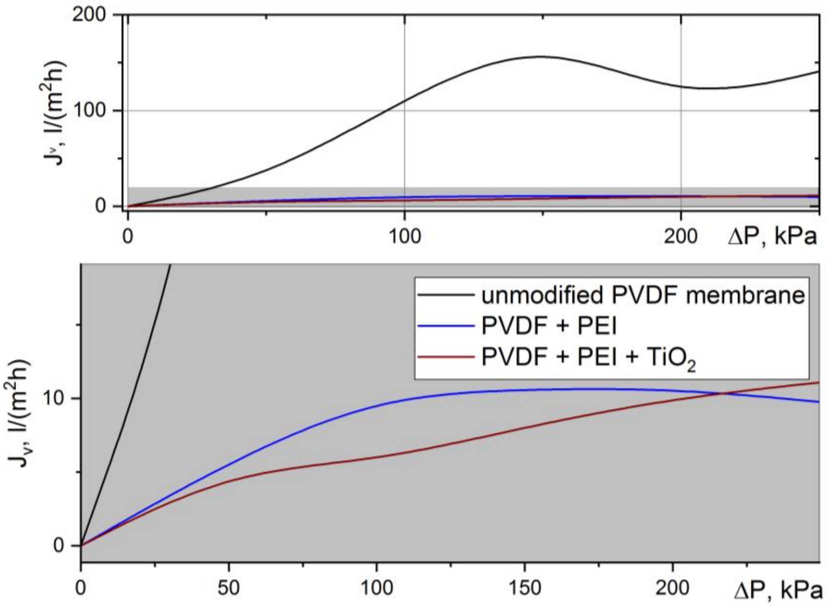

Fig. Dependence of the volumetric flux on an applied pressure for membranes in the process of beer filtration

The unmodified polyvinylidene fluoride membrane was characterised with the highest flux compared with modified membranes, but a dramatic fouling during beer filtration was observed. For membrane, modified only with PEI, decline of the volumetric flux with a pressure increasing was shown because of a concentration polarization. Membrane modified with PEI and TiO_2 nanoparticles demonstrated the linear dependence of the flux on pressure due to photocatalytic properties of titanium(IV) oxide nanoparticles.

Special features for functionalization of carbon nanotubes nanopowders

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The development of methods for the fictionalization of carbon nanotubes nanopowders, determining the patterns of their influence on the physicochemical characteristics is an important task for the creation of new composite materials.

Experimental samples of carbon nanotubes powders (firm “Alit”) of the original and after modifying by pulse treatment with high-voltage electrical discharges (HVED) in a liquid, sedimentation separation, thermochemical and electrochemical reconstruction of the surface were investigated.

It was experimentally found:

- the decrease in the content of amorphous carbon, the average diameter of the granules and the heat resistance of the powder occur: an increase in the specific surface area of the granules of the powder by 5 times of the powder occurs as a result of HVED processing;
- the formation of a powder of three size ranges (0.118–0.139 μm; 2.639–20.895 μm; 2.44–33.701 μm) occurs as a result of sedimentation separation of the powder after HVED processing;
- the increase in specific surface area, total pore volume, micro pores, their average radius, a decrease in the content of impurities occurs as a result of thermo-chemical modifying of the powder;
- the decrease in the content of impurities, free surface saturation energy with water vapor, specific magnetic susceptibility, electrokinetic potential; increasing specific surface area, pore volume, adsorption of the hydrogen occurs as a result of modifying of the powder during electro-chemical processing in a 0.1 N solution of H_2SO_4 in the range of negative potentials of 0.1–0.6 V.

The use of each of the above methods allowed the functionalization of the initial powders, for example, for use as adsorbents of heavy metals.

Consistent application of the methods described above guarantees the manufacture of finely dispersed powders, uniform in size, with a low content of impurities, with a hydrophobic, energy-active surface, suitable for use in the manufacture of abrasive tools.

The investigation into a cytotoxic action of vector magnetic liquids with adsorbed gemcitabine *in vitro*

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The combination of a direct delivery of medicines by means of magnetic nano-particles, an efficient chemotherapy by means of preparations immobilized on their surface as well as immuno therapy with antibodies represents a combinatorial approach, which should evidently provide the most efficient current therapy of corresponding cancer types.

The magnetosensitive colloid systems with an immobilized oncological preparation gemcitabine, conjugated by an antibody CD340 as to HCC tumors have been created.

To determine the effects of experimental combinations on the cells viability of hepatocellular human liver's carcinoma of HepG2 line *in vitro* we studied the samples:

Control:		*Experimental samples:*
Fe_3O_4/ol.Na/PEG	C_{Fe3O4} = 3 mg/ml	Fe_3O_4/oleate.Na/GC
gemcitabine (GC)	C_{GC} = 0.25 mg/ml	Fe_3O_4/oleate.Na/ CD340
Antibody CD340	C_{CD340} = 0.75 mcg/ml	Fe_3O_4/oleate Na/ GC/ CD340
Physiological solution		GC/ CD340

The cytotoxical effects of synthesized magnetic liquids were studied separately for a cytostatic and for an antibody within the colloid system and in a complex.

The efficiency of their cytotoxic action on the cells viability in the line of hepatocellular human liver carcenoma HepG2 has been studied. It has been shown that the colloid system of ML/GC/CD340 causes synergic antineoplastic effect as well as a 20% increase in gemcitabine cytotoxic activity that enables to achieve a cytotoxic effect of a preparation under lower concentrations while diminishing the toxic gemcitabine effect on the organizm as a whole (Table).

Table. Cytotoxic action of synthesized magnetic liquids

Concentration of the experimental combinations			ML	GC	CD340	ML + GC	ML + CD340	ML + GC + CD340	GC + CD340
ML, mg/ml	GC, mg/ml	CD340, mkg/ml	Amount of live cells, % *						
0,1	0,008	0,025	95,4 ± 7,8	78,2 ± 1,6	104,8 ± 3,3	68,7 ± 6,7	85,9 ± 4,3	55,0 ± 5,7	65,7 ± 3,5

The creation of magnetosensitive medical and biological colloid systems with polyfunctional characteristics gives the opportunity to develop the new generation cure.

Magnetically sensitive nanocomposites and magnetic fluids based on magnetite, gemcitabine and HER2 antibody

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The processes of adsorption of gemcitabine (GC) on the surface of nanosized single-domain magnetite (Fe_3O_4) have been investigated. In the experiment conditions, the value of adsorption capacity A was ~ 37.2 mg/g, the extraction degree R (%) – 33.13 %, the separation factor E = 82.58 mL/g. It has been determined that adsorption corresponds to the Freundlich model. Magnetic fluids (MF) were synthesized based on magnetite and physiological solution (PS), stabilized with sodium oleate (OlNa) and polyethylene glycol (PEG), containing GC and HER2 antibody (AB) (Fe_3O_4/GC/OlNa/PEG+PS). The properties of MF were investigated, as well as cytotoxic/cytostatic activity with respect to HepG2 hepatocellular carcinoma of human liver. The synergistic nature of the influence of GC/Fe_3O_4/HER2 complex on HepG2 cells was revealed. It has been determined that IC50 for MF is 0.155 mg/mL, in the range of concentrations of 0.025 - 0.1 mg/mL MF is biocompatible with HepG2 cells. It has been shown that HER2 AB used alone in the investigated concentrations does not affect HepG2 cell viability/proliferation. *In vitro*, GC inhibits the proliferation of liver carcinoma cells, the IC50 value has been 0.02 mg/mL. The use of MF in complex with GC can increase the cytotoxic activity of the composite by 8-10%. The MF+GC+HER2 AB complexes caused the synergistic effect and an increase in the cytotoxic activity, compared with GC used alone, up to 18-20%, while GC contents reduced to 0.008 mg/mL.

The results of the studies indicate that the use of MF based on magnetite, gemcitabine and antibody increases the effectiveness of the antitumor drugs with a significant reduction in their dose and, respectively, the toxico-allergic reactions of the body, and nano-sized magnetite can be promising for the manufacture of magnetically sensitive adsorption materials for medical purposes, e.g. for detoxification of an organism after GC therapy.

On the distribution of crystallite sizes of cerium oxide formed in fumed silica, determined by the WPPM method

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Definition of size parameters of domains or particles of crystalline nanomaterials is usually reduced to computation of crystallites average size from individual diffraction lines on powder diffraction pattern according to methods of Scherrer or Williams-Hall or Warren-Averbach. More complete information on the microstructure of materials can be obtained by using the methods of full-profile analysis of powder diffraction patterns, such as WPPF and WPPM.

In this work, an analysis of the microstructure of CeO_2 formed in fumed silica matrix from $CeCl_3 \cdot 7H_2O$ as a result of heat treatment of composites at different temperatures was carried out. It was shown that in the presence of silica, CeO_2 forms crystallites of a smaller size than in the case of thermal decomposition of one $CeCl_3 \cdot 7H_2O$. The crystallite size of CeO_2 in these composites, calculated by Scherrer, varies from 5 to 11 nm with a temperature change from 400 to 1300 ^{o}C. The fitting of the X-ray patterns of the composites, taking into account their microstructure with WPPM method, were carried out using the PM2K software package [1]. The results of X-ray diffraction processing for composite SiO_2-CeO_2 with 12 wt.% CeO_2, annealed at 800 ^{o}C (Fig., *a*) demonstrate good agreement between the model and experimental curves. Based on the fitted parameters of the log-normal distribution of domain sizes μ and σ, the average sizes of crystallites and their standard deviations were calculated (Fig., *b*).

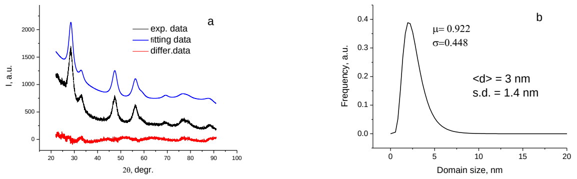

Fig. 1. Results of fitting of model and experimental ddata by WPPM with PM2K program (a) and lognormal distribution of CeO_2 domain sizes (b) for SiO_2-CeO_2, obtained at 800°C

It was shown that as the heat treatment temperature increases, the values of the parameters of the log-normal distribution and the average size of CeO_2 domains also increase. Average crystallite size, determined using the WPPM method, has a smaller value than that calculated by us according to Scherrer [2]. However, from WPPM processing, information on the grade of the distribution of size crystallites of CeO_2 in the silica matrix, depending on the synthesis conditions, can be allocated.

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Composite fillers based on clay/nanosilica blends for cosmetic applications

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Creation of new delivery forms for bioactive substances (BAS) is actual and very important constituent of modern pharmacology and cosmetics. BAS supported on various solids used as delivery systems and providing an increased rate of dissolving of BAS in bioliquids, as well controlled entry into organism or epidermis film.

Supporting materials can longer keep the composition and structure, as well necessary capacity of the BAS loading and kinetics of their delivery. The compositions include clay minerals, pyrogenic silica and diatomaceous earth. The latter has natural origin and composed of both amorphous and crystalline silica and alumina.

In the process of composite creating, components nature and concentrations, different forms of silica and alumina allow one to affect the functional properties of final products. Toothpastes with optimal abrasive properties and medical-prophylactic effects were developed.

The mentioned composite materials were also used to prepare various shampoos. On the base of the investigations, surfactants from coconut oil (Cocamidopropyl betaine, Cocamide MEA, Cocamide DEA), cacao oil (Sodium Cocoabutteramphoacetate), sunflower oil (Sulfosuccinate DNS OD), amphoacetates, *etc.* were introduced into shampoo compositions to add softy influence onto the skin, as well intensification of detergent effect. The applicable compositions of surfactants demonstrate a good compatibility with BAS-composite materials.

Developed samples of the toothpastes and shampoos were produced using an experimental semi-industrial set.

Biopolymer templated hydrotalcite structures

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The present study aimed at investigation of the use of biopolymers, such as starches, in the capacity of templates enabling control over structure and texture of hydrotalcite-like materials.

Hydrotalcites (Ht) of Mg/Al=3 were obtained by co-precipitation at pH=10, using aqueous solution of nitrates as Mg and Al source, and 2 M NaOH + Na_2CO_3, or 25% NH_3aq + $(NH_4)_2CO_3$, as precipitants. The investigated parameters included the type of starch (potato, corn, manioc), starch concentration, starch addition to the selected reagent (nitrates, base, and/or carbonate solution), and temperature of the Ht product washing. The samples were characterized with XRD, SEM, FTIR, TG/DSC.

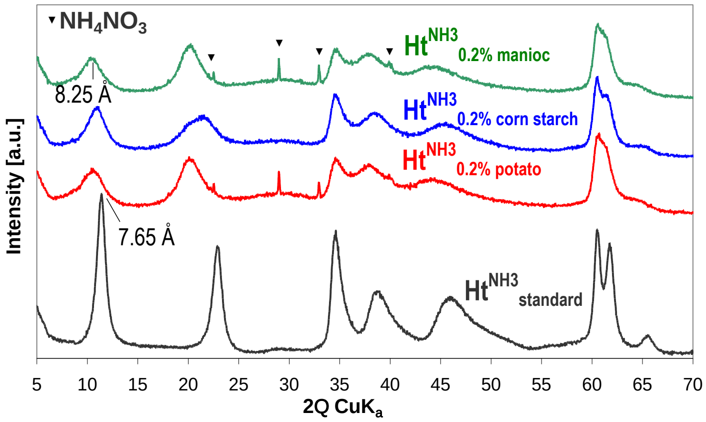

Fig. Effect of different types of starch on the hydrotalcite structure

XRD revealed that starch template facilitates formation of nanocrystalline Ht, as indicated by comparison with the Ht sample obtained by the standard procedure (Fig.). The effect is most pronounced when all reagents used for synthesis contain starch additive. In the presence of starch, the formation of nitrate rather than carbonate forms of Ht is observed. Starch interacts with the Ht material via structural OH, CH_3 and CH_2 groups. Ht obtained in the presence of starch is less stable thermally than the standard reference.

Acknowledgements
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Effect of modification of heteropolyacids with transition metal cations on activity in Baeyer-Villiger oxidation

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Keggin-type heteropolyacids are complex protonic acids possessing very strong acidic properties which can be easily modified through the exchange of the components introduced into molecule structure, such as type of addenda atom, heteroatom or compensating cation [1]. Modification of heteropolyacid structures influences their acid-base and redox properties. The target of our study was the synthesis, physicochemical and catalytic characterization of cobalt salts of tungstophosphoric (HPW) and molybdophosphoric (HPMo) acids having the formula $H_{3-2x}Co_xPX_{12}O_{40}$, where x=½, 1, 1½, and X = Mo or W in the Baeyer-Villiger (BV) oxidation of cylohexanone to ε-caprolactone with molecular oxygen. The Baeyer-Villiger reaction is widely applied in organic chemistry for oxidation of cyclic ketones to appropiate lactones [2]. Oxidation of cyclohexanone leads to the synthesis of ε-caprolactone which is monomer for the production of polycaprolactone [3].

Physicochemical properties of the synthesized compounds were analyzed using different techniques like FTIR spectroscopy, X-ray diffraction analysis and differential scanning calorimetry. Their acid-base and redox properties were studied in the model reaction of ethanol decomposition. All the heteropolysalts were catalytically active in the BV oxidation. The yield of ε-caprolactone and the conversion of cylohexanone were growing with the increase of the metal content in the catalyst molecule. Furthermore, the catalytic activity of cobalt tungstophosphates was higher than the activity of appropriate cobalt tungstomolybdates.

It has been demonstrated that both, acid-base and redox properties of the heteropolysalts, can be considered as key factors influencing their catalytic activity in the studied reaction.

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Laboratory synthesis of N-containing graphene-shaped materials

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Recently, carbon structures modified by nitrogen [1], phosphorus and other adatoms are in the wide demand of scientific research in the creation of functional devices, depending on their intended use.

In this article, nano-dispersed graphene-shaped scales are obtained in the process of synthesis under the conditions of the arc discharge in the medium of nitrogen-containing substances. It was established that by adjusting the power of the arc discharge and the chemical composition of impurities in the medium, it is possible to obtain N-containing materials of various sizes and different surface chemistry in the form of suspensions (Fig., *a*, *c*, *d*) and in dry powdery state (Fig., *b*). Chemisorbed functional groups, which are promising for purposeful adsorption and ion exchange interactions, are obtained due to the impurities' washing and functionalization due to the oxidation of the surface of graphene in physico-chemical and electrochemical processes using hydrogen peroxide.

a *b* *c* *d*

Fig. Graphene-shaped structures:
a) dispersion in water; *b*) powdery dispersion; *c*) hydrophobic (flaming) and hydrophilic parts; *d*) clear water slurry. Tendal's ray (532 nm) in samples *c* and *d*

The spectral and membrane-forming properties of dispersions and suspensions were studied at their use on porous dielectric substrates. It is noted that the conductivity of the membranes may be directed to vary in the range from 10 Ohms to 200 MOhms.

In the laboratory conditions the synthesized materials allow to start a series of studies in primary and secondary sources of current, supercapacitors, sensors, and promising medical biology research.

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Interaction of bio-derived ferulic acid from wheat bran with zeolites seen by TPD MS and FT-IR spectroscopy

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Ferulic acid (FA) is the most abundant phenolic compound in cereals, and it has potential commercial applications in the health, food and cosmetic industries, mainly associated to its antioxidant, antimicrobial, anti-thrombosis and anti-cancer activities [1]. In the wheat bran matrix, its concentration is around ~0.5 wt.%. About 99% of the FA is found in an insoluble bound form, cross-linked with lignin and polysaccharides via ester and ether bonds. This research is focused on the extraction and recovery of ferulic acid from wheat bran using different green hydrolysis strategies (Hot pressurized water, Ultrafast supercritical water, Microwave-assisted hydrolysis, *etc.*) [2] and selective adsorption of free FA from the wheat bran extracts on several commercial zeolites [3].

In this work, temperature programmed desorption mass spectrometry and FT-IR spectroscopy techniques were applied to identify the types of FA interactions with zeolite structures. Samples of FA on the surface of zeolites obtained by various methods, including adsorption from the hydrolysed wheat bran extracts were investigated. The presence of several functional groups in the FA molecule (methoxy, carboxyl and phenolic groups) leads to the formation of several types of surface complexes. The interaction via the phenolic group prevail at low concentrations of FA. However, an increase of the FA concentration, promotes the number of complexes bound through the carboxyl group.

Acknowledgements
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Synthesis of nanosized magnesium and copper(II) phosphates and polycrystalline silver phosphate

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It is known that silver or copper(II) phosphates, when studied separately, act as catalysts of paraffin, isomerization alcohol oxidation to aldehydes [1,2] while double phosphates of these metals are advanced materials for functional use [3]. The potential for cobaltous phosphate use as catalyst in electrochemical process of hydrogen production from water is demonstrated in [4], which is of practical importance for hydrogen energetics. It can therefore be said that phosphates of other *d*-metals will also exhibit similar properties. Mixtures of nanosized magnesium or copper(II) phosphates and polycrystalline silver phosphate have been obtained from aqueous solutions of silver and magnesium or copper(II) nitrates and sodium hydrogen phosphate at basic mixture ratios $[AgNO_3]:[Me(NO_3)_2]:[Na_2HPO_4] = 1:1:1.7$ (Me – Mg, Cu) and temperature of reacting solutions 80 – 90°C. The codeposited silver and magnesium phosphates and silver and copper(II) phosphates have been studied using chemical, thermogravimetric and X-ray diffraction analyses. It has been shown that the particles of magnesium and copper(II) phosphates have nanosize, in particular up to 100 nm. In parallel, the deposition of polycrystalline cubical silver phosphate from aqueous solutions has been observed under the same conditions. Heating of the mixture of coprecipitated silver and copper(II) phosphates to more than 417°C (and up to 720°C) resulted in the formation of double phosphate. The temperature intervals of dehydration, crystallization of X-ray amorphous phases and interaction of silver and copper(II) phosphates with the formation of double phosphate have been established. The obtained compositions of silver and magnesium or silver and copper(II) phosphates are of practical importance. They have been tested as catalysts for the separation of hydrogen from water, isomerization of hydrocarbons or oxidation of alcohols to aldehydes.

The materials on the basis of obtained mixtures contain biologically active elements, and therefore can be used in the production of water filters and functional materials for biosystems.

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The influence of external surface modification on the zeolite catalysts coking

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Some dealumination agents under certain conditions act primarily on the external surface of zeolite microcrystals [1-3], which leads to the loss of its active sites. Therefore this can serve as a fuse for the carbon deposits formation and their accumulation at the entrances to zeolite cavities because the reaction in this case is redirected into the inner space of the micro crystals. It should be noted that coke formation is the main reason of the loss of catalytic activity, at least on acidic zeolite catalysts, which is especially manifested in the cracking reaction. This occurs precisely with the participation of acidic sites with the formation of a large number of unsaturated hydrocarbon molecules. At the same time, deactivation by coke is poorly investigated for basic catalysts.

The aim of this work is establishing the influence of external surface dealumination on coking the zeolite catalysts of different types and revealing the nature of coke formed in the basic zeolite. The catalytic method, chromatography, FTIR spectroscopy and were supplied in the investigations.

It was found for the acidic catalyst of cracking of olefins that the coke formation begins inside the zeolite cavities, since deactivation of the external surface is not crucial for saving its cracking activity. Whereas the modification of the basic catalyst of toluene with methanol alkylation using $(NH_4)_2SiF_6$, besides the increase in its selectivity to styrene and ethylbenzene [4, 5], leads to its more stable work while coke formed for the most part on the external surface of the catalyst. The main role in deactivation of the latter was shown to play the polynuclear aromatic coke.

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Formation of tryptophan complexes with silver and copper nanoparticles on the surface of tissues with stable bactericidal action

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Biomedical preparations with pronounced bactericidal properties based on cotton tissue modified with nanoparticles (NPs) of silver and copper with size 20-60 nm have been obtained. The stable and reliable bactericidal activity of modified fabrics (assessed by the inhibition zone of bacterial growth) was evaluated against bacteria *E. coli*, *K. pneumonia*, *P. aeruginos*, *S. aureus*, *E. faecalis*. To suppress a toxic effect of nanoparticles we investigate the possibilities of adsorption modification of Ag- and Ag/Cu-tissues by amino acid tryptophan (Trp). Adsorption of Trp on the surface of bactericidal tissues occurs due to complexation with the corresponding ions, the source of which are Ag and Cu NPs. Isotherms adsorption of tryptophan demonstrate a significantly higher adsorption capacity of Ag/Cu/tissue compared to Ag/tissue. The high adsorption capacity of the tissue with bimetallic Ag/Cu NPs in comparison with Ag NPs is explained due to possible formation of a bidentate complex of copper $Cu(Trp)_2$. The effect of the type of complexes on the desorption of ions upon contact of the modified tissue with water was studied. Approximately 20% of silver ions are released from the surface of the Ag/Trp/tissue, and in the presence of a bimetallic composite, the ions of silver and copper are firmly held by the tissue. The release of ions from the surface of the NP in the presence and absence of Trp is markedly different. Metal ions are firmly held inside the complex on the surface of the fabric. The paper discusses the mechanism of the formation of complexes and their interaction with the surface of tissue containing glycosidic residues and OH groups. It is shown that the complexation of NPs with Trp on the surface of tissues does not affect their pronounced bactericidal action against to a number of microorganisms.

Bifunctional iridium electrocatalysts for modifying surface of fuel cell proton-conducting membranes

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Currently, fundamental and applied researches are directed on the development of fuel cells and electrolyzers with using highly-efficient electrocatalysts and proton-conducting membranes. Both these devices can be combined in unitized regenerative fuel cell (URFC) [1,2]. The main problem in the development of URFC is the synthesis of stable nanosized high-performance bifunctional electrocatalysts for both oxygen reduction and oxygen oxidation electrode reactions. The most stable and efficient electrocatalysts are based on 5*d*-metal iridium. Researches in this field is too expensive due to using precious metals and Nafion membrane. Therefore, it is important to use minimum quantity of iridium with maximum effectiveness.

The aim of this work was to develop a synthesis of nanosized highly-efficient bifunctional iridium catalyst for oxygen electrodes of URFC and method for its application onto the Nafion membrane.

Iridium nanosized catalysts were prepared using hexachloroiridic acid and sodium borohydride as a reducing agent. Synthesis was carried out in an alkaline solution of ethylene glycol while stirring continuously until the hydrogen evolution was stopped. Polyvinylpyrrolidone was used for regulation of iridium particle size. At polyvinylpyrrolidone concentration of 0.2 % the particle size was 2-3 nm but at concentrations of 0.6-1.2 % the particle size was 1.5-2 nm. The obtained electrocatalysts were applied on the surface of the membrane in the form of catalytic inks made on the basis of the Nafion monomer. Heat treatment at 130 ºC was made after application. These catalysts showed high performance at oxygen electrodes of fuel cell and electrolyzer in the URFC .

Thus, the method for manufacturing nanosized iridium electrocatalysts has been developed. After application on Nafion membrane they demonstrated high performance as bifunctional oxygen electrocatalysts in URFC.

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Synthesis of nanostructure yttrium-aluminum garnet powders activated with cerium, europium, gadolinium and their luminescent characteristics

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A progressive method of luminescent nanostructure yttrium-aluminum garnet powders doped with rare-earth ions was developed. This method based on the nitrate salts combustion in the presence of complex organic fuel (urea and hexamethylenetetramine). The modes of synthesis are optimized and structural and spectral-luminescent characteristics of the ultradispersed powders of chemical composition $Y_3Al_5O_{12}$:Ce, Eu, Gd with the sizes of 0.8-1.2 μ are studied. The nanostructure powders were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), and IR-spectroscopy. The components $Y(NO_3)_3{\cdot}6H_2O$; $Al(NO_3)_3{\cdot}9H_2O$; $Ce(NO_3)_3{\cdot}6H_2O$; $Eu(NO_3)_3{\cdot}6H_2O$; $Gd(NO_3)_3{\cdot}6H_2O$; $CO(NH_2)_2$; $(CH_2)_6N_4$ are mixing in distilled water. The solution is concentrated in the oven at 80 – 100 ºC to obtain the gel and is heat-treated in muffle furnace at 1100 ºC. The spectral-luminescent characteristics depend on concentration and nature of doping impurities, temperature of heat treatment, and type of organic fuel. Doping of yttrium-aluminum garnet with cerium at excitation 440 nm causes broadband luminescence in the range of 480 – 700 nm, additional powders doping with europium leads to curve shift in longer wave length and appearance additional band 610 nm on curve, belonging of europium ions emission. Doping of yttrium-aluminum garnet with cerium and gadolinium at excitation 440 nm leads to curve shift in longer wave length too (during firing in the air at 1100°C in all cases). $Y_3Al_5O_{12}$:Ce, Eu, Gd phosphors prepared through combustion reaction under controlled condition can be applied in light emission diodes source with emission of warm white light.

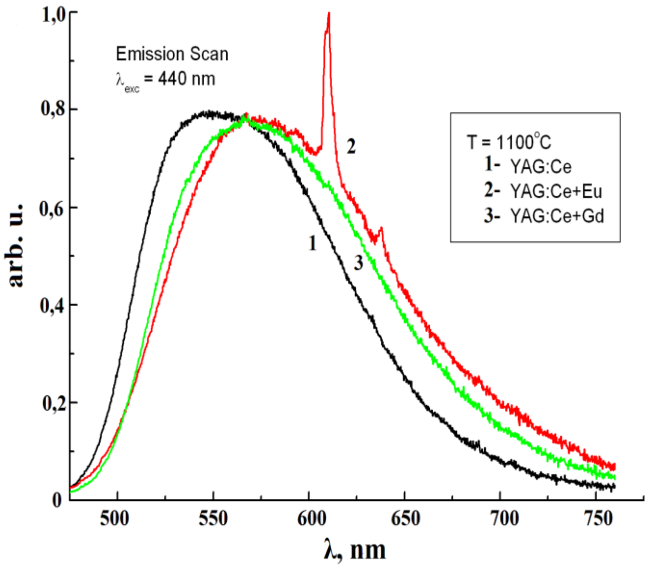

Fig. Luminescent spectra $Y_3Al_5O_{12}$:Ce,Eu,Gd

Stationary and quasistationary electron states in quasiatomic nanosystems

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In study[1] we find that the binding energy of an exciton formed from an electron and a hole spatially separated from each other (the hole is moving within a quantum dot (QD), and the electron is localized above the spherical QD – matrix interface) in a quasiatomic nanosystem containing semiconductor (germanium) and insulating (aluminium oxide) QDs is substantially increased (by nearly two orders of magnitude) compared to the exciton binding energy in a silicon and aluminium oxide single crystal. It is established that, in the band gap of an germanium and aluminium oxide QDs, there is a band of exciton states (formed from a spatially separated electron and hole). It is shown that there exists the possibility of experimentally detecting the ground and excited exciton states in the band gap of an germanium and aluminium oxide QDs at room temperature from the absorption and transmittance spectra of the nanosystem. The effect of a substantial increase in the exciton binding energy offers considerable scope for the use of insulating nanoheterostructures as the active region of nanolasers operating at excitonic transitions [1].

The theory of excitons from spatially separated electrons and holes (the hole moves in volume QD, and the electron is localized over the spherical surface boundary of (QD/matrix)), developed in [2,3], for the case in which centrifugal energy of the electron is considered in the potential energy of the exciton. It has been shown that the taking into consideration centrifugal energy in the potential energy of the exciton leads to the occurrence of the quasi-stationary states in the band of the surface exciton states, which with the increase of QD radius transfers into stationary state. It is established that the light spectrum of the interband absorption (emission) of nanosystems consisting of the energy bands which are formed by the electron between quasi-stationary and stationary states, and intraband absorption spectra – from the bands caused by electron transitions between stationary states [2,3].

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Ways to improve the corrosion resistance of fuel cladding materials of light-water nuclear reactors

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The growth in electricity demand worldwide with the need of managing greenhouse gas emission explains continuing interest in developing nuclear power generation. The vast majority of modern reactors are light water reactors. In all of them uranium oxide (UO_2) is sintered into fuel pellets and then encased in ~4-m-long metal tubes (fuel cladding) made of Zr-based alloys.

The materials inside the core are exposed to an extremely harsh environment due to the combination of high stress, high temperature, a chemical aggressive coolant, and strong radiation. The fuel cladding is the first full barrier for retention of radionuclides and thus comprises one of the most important components of plant safety. For a long time primary materials for fuel cladding consist of Zr-based alloys. However, their satisfactory performances are challenged once the local environment changes from normal operating conditions to design-basis (DB) or beyond DB ones. Last such example was the severe nuclear accident at the Fukushima power plant in March 2011.

This explains the motivation for modification or transition away from Zr-based fuel cladding to decrease the rate and total amount of heat and hydrogen generated in high temperature steam that offers improved coping time under accident conditions. Now several opportunities for this are considered:

1) Application of conventional surface modification techniques, such as ion implantation or plasma electrolytic oxidation.

2) Adoption of a protective coating on the surface of Zr-based alloys. It is known that materials capable of exhibiting high temperature steam oxidation resistance are chromia, alumina, and/or silica formers. Therefore, any protective coating needs to contain at least one of the elements Cr, Al, or Si.

3) Developing oxidation-resistant monolithic or layered cladding materials, such as Fe-based alloys, SiC composites, and multilayer Mo cladding. In this respect the Fe-Cr-Al alloy class looks very promising because it has been widely used in many industries where high temperature oxidation resistance is needed including vapor containing environments in fossil fuel energy plants.

In report short review of current situation in this area is presented. Special attention is given to Fe-Cr-Al alloys consisting of Cr and Al dissolved in BCC Fe lattice, which stabilize the BCC structure to the melting point of the material (~1500°C). These alloys possess high-temperature strength and excellent oxidation resistance. The Pourbaix diagrams which allows to determine the possibility of corrosion with hydrogen or oxygen depolarization is estimated.

Electrophysical properties of polychlorotrifluoroethylene nanocomposites based on calcium iron oxide modified with copper sulfide

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The magnetic oxide nanoparticles are of significant interest due to their wide applications, ranging from fundamental research to industrial use. The interest in the nanoferrites is because of their important physical and chemical properties. They were used in many fields such as making microwave devices, catalysts, antenna materials high frequency transformer core, and magnetically-guided drug delivery devices. Calcium ferrite has shown high potential for applications to oxide semiconductor *p*-type photoelectrodes, catalytic agents, magnetic materials and gas sensors.

$CaFe_2O_4$ nanopowders were synthesized by the sol-gel auto-combustion method. The formation of orthorhombic $CaFe_2O_4$ compound was confirmed by X-ray diffraction (Fig., *a*). To grow of CuS onto $CaFe_2O_4$, a typical procedure was as follows. $CaFe_2O_4$ were treated with CTAB solution. Then the $CaFe_2O_4$ were washed by water and redispersed into Na_2S aqueous solution. The above solution was stirred at room temperature for 3 h. Then the copper sulfate aqueous solution was added dropwise into the above Na_2S aqueous solution and stirred for 3 h. The samples of system $CuS/CaFe_2O_4$–polychlorotrifluoroethylene (PCTFE) was compacted at the temperature equal to the melting point of the polymer at a pressure of 2 MPa.

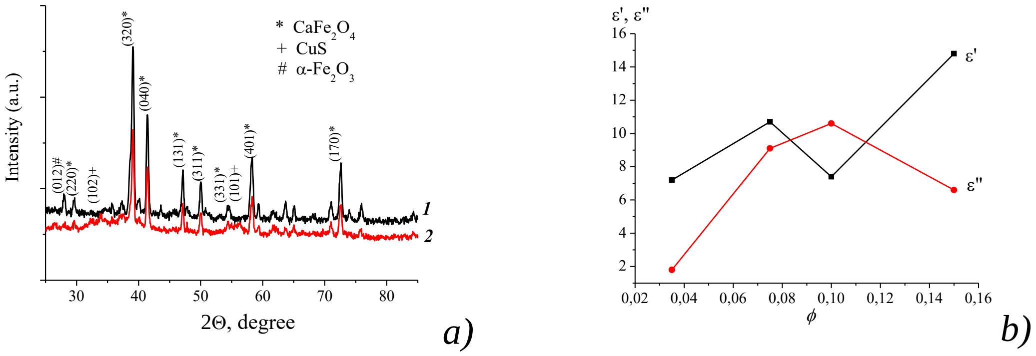

Fig. X-ray diffraction patterns of synthesized nanoparticles: *1* – $CaFe_2O_4$, *2* – $0.32CuS/CaFe_2O_4$ (*a*), dependence of ε' and ε'' at a frequency of 9 GHz polymer nanocomposites by volume content (ϕ) of copper sulfide in systems $0.32CuS/CaFe_2O_4$– PCTFE (*b*)

The real (ε') and imaginary (ε'') components of the complex dielectric permittivity (Fig., *b*) of conducting composites at microwave frequencies (range 8-12 GHz) were measured using the interferometer by an electrodeless method.

Synthesis and properties of nanostructures absorbing ultrahigh-frequency electromagnetic and neutron radiation

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NiCo nanoparticles were obtained on the surface of oxidized and nonoxidized multi-wall carbon nanotubes by the method of chemical precipitation of nickel and cobalt carbonates from a solution of hydrazine hydrate. Real and imaginary components of the complex dielectric and magnetic permeability were determined for dispersed NC samples. $CoFe_2O_4$ and $NiFe_2O_4$ ferrites with a nanoparticle size of 30-50 nm were synthesized by sol-gel autoburning method. When modifying the surface of ferrites with copper iodide, nonlinear concentration dependences are observed for the values ε', ε'' in the microwave range and conductivity values (σ) at low frequencies. After putting of the modified NC into polychlorotrifluoroethylene (PCTFE) there is an increase in these electrophysical parameters at room temperature. The real and imaginary components of the complex dielectric permeability of the samples of $CuI/CoFe_2O_4$-PCTFE system are 3-5 times higher and the electrical conductivity is 1-2 orders higher than that of the $CuI/NiFe_2O_4$-PCTFE system. According to magnetic measurements, the thickness of hematite layer formed on the surface of ferrite, which affects the saturation magnetization of ferrite, is calculated to be ~ 1.5 nm for $NiFe_2O_4$, and for $CoFe_2O_4$ ~ 2.9 nm. The change in the thickness of this layer can be controlled by the electrophysical properties of composites based on $CuI/CoFe_2O_4$ and $CuI/NiFe_2O_4$. The model of polyfunctional NC of superparamagnetic core – multilevel shell type in composition of a magnetic fluid was analyzed. The interconnection of magnetic properties and size parameters was investigated for synthesized multilevel nanostructures. Using experimental data and calculations, the shell structures were optimized for the specific surface area, the number of layers, the size distribution of NC particles, the stabilization layer parameters, and so on.

The synthesized NC are promising for creation of matrix-dispersed materials, effectively absorbing ultrahigh-frequency electromagnetic and neutron radiation; and MF – for use in medicine as means of targeted delivery, local therapy by neutron capture method and diagnostics in real time.

Composites based on layered double hydroxides – sorbents for the recovery uranium(VI)

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The presence of U(VI) in natural waters, predominantly in the form of negatively charged di- and tricarbonate-uranyl complexes, greatly complicates its extraction from aqueous media and eliminates the sorption of U(VI) on the surface of mineral and organomineral suspensions. Prospective are magnetic nanocomposites based on layered double hydroxides (LDH) intercalated with citrate ions ($C_6H_5O_7^{3-}$). The inclusion of organic reagents in the interlayer space increases their selectivity to U(VI) by increasing the concentration of reaction centers in the matrix of sorbents, since citrate ions form strong chelate complex compounds with many ions of toxic metals [1].

Isotherms of sorption of U(VI) at the pH of the aqueous solution of 5.0, V/m = 500 cm^3/g and sorption duration of 1 hour on composite sorbents – magnetic citrate forms Mg/Al- and Zn/Al-LDH are obtained. They have been processed in accordance with the Langmuir equation, which is the most commonly used for description of adsorption in solid phase-liquid phase systems. The correlation coefficients are ($R^2 > 0.9$). In the wide range of the initial concentration of U(VI) (50-600 μmol/dm^3), a gradual saturation of the surface of the LDH is observed. The calculated value of the U(VI) maximum adsorption for Zn/Al- and Mg/Al-LDH magnetic compositions is 92.6 and 97.1 μmol/g, respectively. The removal of U(VI) on the sorbents under study occurs due to the formation of complex compounds with $C_6H_5O_7^{3-}$ ions in the interlayer space of the LDH, due to the binding of U(VI) to hydroxyl groups on the surface of brusitoid-like layers and the ferinol groups of magnetite, as well as the isomorphic substitution UO_2^{2+} ions for Zn(II)/Mg(II) in the LDH.

Thus, in the work, the sorption ability of composites based on LDH is established for the purification of aqueous media from compounds of U(VI). Providing such sorbents with magnetic properties will reduce the technological costs of separating formed sludges from the liquid phase and ensure the safety of personnel during decontamination of liquid radioactive waste.

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Development of multifunctional enzyme-bearing magnetic nanocomposites

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A growing problem of drinking water pollution by pharmaceuticals has arose in modern society. Contents of persistent organic pollutants such as pharmaceuticals, personal care products, and their metabolites drastically increased due to the human activity. Common features of water treatment methods such as UV-treatment and ozonation are high energy consumption and production of potentially toxic and even, carcinogenic byproducts. Taking into account disadvantages of the above-mentioned methods, enzymatic water treatment can be proposed as an attractive alternative solution.

Developed methods for enzymes immobilisation on magnetite/silica surface and the activity of composites in model solution were evaluated. Synthesized magnetic nanocomposites with advanced biocatalyst library including *Jack Bean Urease*, *Trametes Versicolor Laccase*, *Horseradish Peroxidase* and *Lignin peroxidase* were thoroughly characterized using FTIR, TGA, SEM, AFM, UV-Vis, NMR, MALDI and enzymatic assays methods.

Immobilized enzymes demonstrated high performance in drug decomposition tests, even in presence of typical inhibitors, namely Cd(II) and Cu(II) ions. For instance, urease enzyme immobilized onto Fe_3O_4/SiO_2-DTPA composites revealed high activity during 18 cycles of urea decomposition [1, 2]. As another example, chemisorbed laccase retained up to 100% activity in 50 oxidation cycles of model compound – ABTS, even in the presence of Cd(II) ions [3]. Sol-gel entrapped lignin and horseradish peroxidases were active in diclofenac, acetaminophen and carbamazepine drugs' transformation.

All the composites showed high adsorption capacity towards heavy metals ions along with drug decomposition performance. Thus, synthesised materials could be used for complex water purification from cocktail mixtures of medicines and heavy metals.

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Comparison of the influence of hydro-and alco-thermal treatment on the structure of zirconium silicate

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Zirconia-Silica aerogels with high porosity and high specific surface, low density and low thermal conductivity, strong energy of Zr-O-Si bind can serve as excellent sorbents, catalyst carriers and thermoinsulating materials. In this work, an attempt was made to obtain Zr-Si–aerogels from spherically granulated hydrogels synthesized by the direct sol-gel method by alternating their hydrothermal, alcohol, and alco-thermal treatments. The thermal stability of the samples was evaluated by the change in their structural-adsorption properties after calcination in air. The results are shown in the Table.

Table. Parameters of spherically granulated gels 0.6 ZrSi after various treatment

Preliminary processing	S_{BET}, m^2/g	V_{pore}, cm^3/g	R_{pore} average, Å	$R_{pore\ DFT}$, Å	W, g/cm^3	S_{BET}, % wastage
Drying at 130 °C	389.3	0.255	13.08	12.52	1.33	
Calcination at 600 °C	219.9	0.158	24.43	14.39		43.51
HTT* at 270 °C, 5 h. Drying at 130 °C	517.5	0.597	23.07	28.41	1.05	
HTT at 270 °C, 5 h. Drying. Calcination at 600 °C	414.7	0.49	31.2	35.16		19.86
HTT at 270 °C, 2 h. Ethanol. Drying at 130 °C	540.8	1.154	42.68	47.08	0.402	
HTT at 270 °C, 2 h. Ethanol. Drying. Calcination at 600 °C	450.28	0.835	45.56	47.08		16.59
HTT at 270 °C, 2 h. Ethanol + 2 % petrol. Drying at 130 °C	549.1	1.975	71.95	126.2	0.264	
HTT at 270 °C, 2 h. Ethanol +2 % petrol Drying. Calcination at 600 °C	485.8	1.806	74.38	136.9		11.53
ATT** Ethanol +2 % petrol at 270 °C, 5 h. Drying at 130 °C	511.0	2.258	88.38	136.9	0.221	
ATT Ethanol +2 % petrol at 270 °C, 5 h. Drying. Calcination at 600 °C	494.3	2.000	91.48	136.9		3.27

*- hydrothermal treatment; **- alcothermal treatment

It is shown that strengthening the gel structure by its HTT contributes to the growth of the surface area, volume and width of pores and more than doubles its thermal stability. Additional decantation with ethanol leads to a substantial increase in the volume and width of the pores, an increase in thermal stability of the samples, and reduces their density, even with a shorter duration of the HTT. The introduction of petrol impurities into ethanol, and even more ATT of samples in this mixture, leads to production of thermostable materials with a density < 0.3 g/cm^3, which is characteristic of metal oxide silica aerogels.

Modified citric method for obtaining of functional oxide materials

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The work is devoted to the actual topic – synthesis of nanomaterial on the base of transition metal oxides using the citric acid routes. Among other chemistry approaches, these routes are simple, employ cheap reagents, and enable one to obtain target products, which are free of impurities, have the uniform size distribution of particles, and possess great surface area and developed porosity.

The main our efforts have been directed towards elaboration of a modified citric acid aided route for the synthesis of various oxides for sorption, catalysis and electrochemical applications. As decomposition of citrate precursors implies numerous steps including dehydration and formation of aconitates and itaconates, similarities and differences in decomposition schemes and morphology of oxides obtained are analyzed and discussed, an optimal metal to citric acid ratio is suggested, and possible presence of higher (or lower) oxidation states in target compounds is analyzed in terms of thermodynamics of red-ox processes involving oxygen and carbon monoxide formed when the organic part of precursors decomposes. Based on this analysis, possible improvements of the citric acid aided route are suggested.

Examples include synthesis [1-7] and testing of catalysts for volatile organic compounds (VOC) oxidation [2], numerous electrode materials for lithium batteries of high power, like $LiMn_2O_4$ [3] and $LiNi_{0.5}Mn_{1.5}O_4$ [4], $LiFePO_4$ [5] and $Li_4Ti_5O_{12}$ [6], and silica gels modified by Fe_2O_3 [7] for the sorption of phosphates.

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Antiviral properties of nanoparticles from the physical point of view

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There are many experiments demonstrating antiviral activity of non-functionalized nanoparticles, but there is no unified view on the interaction between the nanoparticles and viruses, which could explain all the features of this action. The idea of physical reasons of antiviral activities of non-functionalized nanoparticles against various viruses is proposed.

The main reason of antiviral activities is the near-field interaction between the virus and the nanoparticle. We show that the features of antiviral action of nanoparticles are similar to some features of near-field interactions. Namely, the local-field enhancement is the reason of the hot spots (the domains of enhanced local field and high field gradients, see Fig.) at the virus surface molecules which lead to distortions of the molecules. The distortions prevent the virus binding, its entry or membrane fusion, i.e. the virus cannot infect the living cell. Simulation of the interaction between the virus and the nanoparticle in the framework of the proposed idea allows explaining existed experimental results obtained by different research groups and predicting further experiments. These results allow us to state that near-field interaction between the virus and the nanoparticles may be the reason of antiviral action of the nanoparticles.

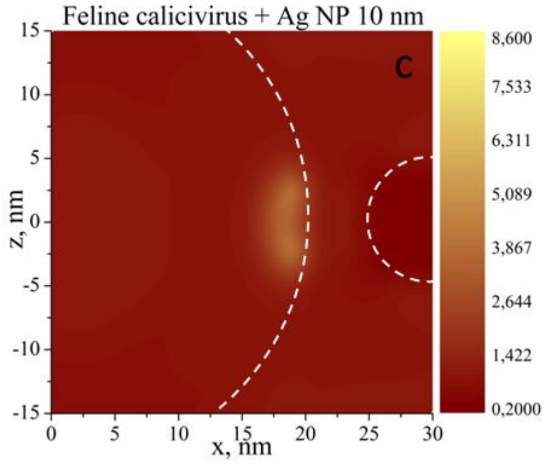

Fig. Local field distribution in the system of virus and nanoparticles demonstrating the “hot spots” on the virus surface

Coal transformation into nanoporous carbon under heat-shock alkali activation

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The aim of the work is to establish the regularities of brown coal transformation into nanoporous carbon during heat-shock alkali activation.

Transformations were evaluated by changing the properties of thermolysis solids (TSs) with increasing heat-shock temperature t_{HS} up to 800°C. The TSs preparation included 1) the rapid introducing of sample (coal+KOH) into reactor preheated to t_{HS} varied within 400-800°C, 2) isothermal exposure at t_{HS} (1 h), 3) washing from KOH and drying. The TSs structure was studied by X-ray diffraction, FTIR-spectroscopy and nitrogen adsorption (77K). Based on N_2 adsorption-desorption isotherms, the pore size distributions, the volume (V) and the specific surface area (S) of adsorbing pores, the V and S values of macro- (V_{ma}), meso- (V_{me}) and micropores (V_{mi}), as well as subnanopores (V_{1nm}) – pores with an average width of $W \leq 1$ nm were determined.

The main reactions at $t_{HS} \leq 400$°C were established to be the elimination of polyarenes substituents and C-O, C-C bonds heterolysis splitting the coal framework into fragments being precursors of the secondary porous framework of NC. When t_{HS}=400-800°C, the TSs porosity is formed on the background of condensation reactions leading to 1) an increase in the polyarenes sizes without aggregation into crystallites and 2) the formation of spatially disordered polyarylene structures. A t_{TS} increase was established to result in the forming TSs with increasing S from 14.7 m^2/g (400°C) to 1947 m^2/g (800°C). The V value increases in 7.2 times (from 0.124 to 0.892 cm^3/g). The main growth of pore volume is due to micropores: the V_{mi} values increase from 0 to 0.547 cm^3/g, the subnanopores contribution becomes dominant (84-98%) at t_{HS}=600-800°C. Pores with $W \leq 5$ nm were found to develop most dynamically under cooperative action of KOH and heat-shock. Pore size distributions are characterized by maxima corresponding to subnanopores (dV_1), micropores with W=1-2 nm (dV_2) and mesopores with W=3-5 nm (dV_3). The dV_1 value grows exponentially with increasing t_{HS} (R^2=0.988) that allows to evaluate some parameter (56.1 kJ/mol) which is formally similar to the activation energy and characterizes the t_{HS} influence on the $V_{1\ nm}$ volume increment with increasing width. A heat-shock is concluded to promote the 1 nm pores formation limited by the diffusion of the activator (KOH or K atoms as the products of K^+ ion reduction) within the forming three-dimensional framework of nanoporous carbon.

The study of photocatalytic properties of doped tin oxide prepared by sonochemical method

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There are several ways to improve the activity of photocatalysts active under the action of visible light: phase and morphological control, doping, composite material. Tin dioxide is one of such semiconductors-photocatalyst. However, the question of the effect of one of these methods - the doping on photocatalytic properties of SnO_2 under visible light irradiation insufficiently studied. We studied sonochemical treatment (UST) of heterogeneous and homogeneous precipitation gels of SnO_2 in the presence doping additives of *d*- and *f*-metals in the form of salts and oxides (0.5-5% by weight on oxides). The changes in porous structure, electronic characteristics and photocatalytic activity of SnO_2 due to UST and doping have been studied.

The initial samples are microporous. The doped samples SnO_2 have porous structure with low the proportion of micropores in the total pore volume. The formation of meso-macroporous structure is observed. Thus, the porous structure of doped samples becomes more open and accessible to dye molecules.

The absorption edge for initial SnO_2 is 296 nm which corresponds to band gap E_g = 4.19 eV. After UST, these characteristics don’t change. But, under UST with the introduction of dopants, there is a bathochromic shift of absorption edge. As a result, the band gap band is narrowed almost twice. For example, when doping with silver, E_g is 2.65 eV, when doping with titanium - 2.9 eV, while when using molybdenum oxide as a dopant, it is 3.1 eV. In addition, the absorption of visible light increases to 40-50% compared with un-doped samples. Most likely, this is related with the creation of new energy levels in the band gap what happens at the introduction of doping additives. All doped specimens have a higher photocatalytic activity in the processes of degradation of dyes with visible irradiation compared to the initial samples. SnO_2, doped with silver, exhibit maximum photocatalytic activity. The K_d values achieve 10^{-3}-10^{-4} s^{-1}.

Synthesis of Ti-containing photocatalyst supported on stainless steel

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The supported Ti-containing catalyst on a surface of stainless steel foil was prepared by low temperature ion implantation method. The high photocatalytic activity of this catalyst in the process of neutralizing benzene in aqueous solutions under irradiation with visible light, which significantly exceeds its activity in the UV range was shown. The surface composition and the effect of calcination temperature were characterized by XRD, SAXS, SEM, AFM, and XPS. It was shown that after ion implantation on the surface of a stainless steel, a nanosized layer of the implant was formed. Presence of titanium oxide, nitride and oxynitride was determined by XPS method. Increasing the calcination temperature leads to decreasing the samples activity and can be explained by the influence the ratio between the nitride, oxynitride and oxide phases of titanium. Exactly the presence of those phases on the surface explains its high activity in the degradation of aqueous benzene solution under visible light irradiation. Thus, using of the obtained samples in the degradation of aqueous benzene solutions under visible light irradiation is perspective from ecological point of view.

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Active carbons from nutshells – preparation, properties and application

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Currently, one of the leading research trends is obtaining and applying the adsorbents from waste raw materials [1-3], which is part of the principles of green chemistry.

The aim of these studies was to obtain a series of carbon materials using waste materials of vegetable origin, as well as to determine their structural and surface properties, and to assess their suitability in the processes of water and wastewater treatment.

A series of carbon materials from shells of walnuts was obtained by pyrolysis at various temperatures. The adsorbents were modified by impregnation with various reagents. The structural properties of obtained adsorbents were determined by low temperature measurements of nitrogen adsorption/desorption isotherms and electron microscopy (SEM, TEM). In order to estimate the potential use of obtained materials in the processes of removing impurities from solutions, their adsorption properties were determined. Therefore, the measurements of equilibrium and kinetics of adsorption of selected aromatic organic compounds from the group of dyes, pesticides and nitrophenols were conducted. The obtained equilibrium data were analyzed by using the simple isotherm equations relating to adsorption on energetically heterogeneous solids. The received profiles of changes in concentration over time were fitted using simple equations of adsorption kinetics including: PFOE, PSOE, m-exp, MOE, f-MOE and diffusion models (IDM, PDM). The analysis of obtained results allowed the selection of optimal conditions for conducting the pyrolysis and modification processes in the context of obtaining an effective adsorbent for waters and wastewaters purification.

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Active carbons with pharmaceutical use: structural and adsorption properties

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Active carbon is a material mainly used as a medium for adsorbing chemical substances. It consists of elemental carbon in the form of amorphous soot and partly in the form of fine graphite. However, it also contains ash, alkali metal oxides and silica. Active carbon is characterized by good mechanical properties and expanded porous structure, which makes it an excellent adsorbent for many substances [1-3]. In addition, it is non-toxic, cheap to manufacture and easy to dispose of [4-8]. Currently, due to the huge raw material base, well-known production methods and valuable properties of activated carbon (which may vary and can be modified depending on the direction of potential use of this material), the area of its application is constantly growing. Currently, its widespread use includes the chemical industry, electronics, various vacuum technologies, removal of pollutants from water and sewage, medicine (treatment of diarrhea, indigestion and flatulence, drug poisoning and others) [1-3].

The aim of this work was to compare the properties of active carbons of pharmaceutical use. Based on the measurements of nitrogen adsorption/desorption isotherms the structural properties of selected adsorbents were estimated. The adsorption effectiveness of these materials towards the aromatic organic compounds was determined basing on the equilibrium and kinetic measurements. The data obtained were analyzed using simple equations and models of adsorption equilibrium and kinetics.

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Mesoporous metal oxide anodes for Li-ion batteries

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Lithium-ion batteries are today most attractive rechargeable batteries due to high energy storage per unit volume and weight. However, their performance still needs further development for use in high energy density applications, e.g., cars and large scale energy storage. Thus an important direction is improvement of anode materials. Tin oxide is a material that attracted a lot of interest because of its high theoretical capacity. It was demonstrated that mesoporous anodes composed of nano sized SnO_2 particles (NP) show substantially higher specific capacities, rate performance, coulombic efficiency, and cycling stabilities compared to available commercial tin oxide. A discharge capacity of 778 mAh/g, close to the theoretical limit of 781 mAh/g, was achieved [1].

Investigation of NP tin oxide at different cycling conditions and higher temperature could extract more than the theoretical capacity. All initial capacities in this case show values above 1600 mAh/g, due to formation of soluble electrolyte reduction products and partial dissolution of solid electrolyte interphase species. The most stable behavior over 120 cycles was obtained at room temperature or at cycling with a fast rate at elevated temperature.

To make batteries cheaper and more environmentally friendly, materials with low toxicity, abundant in the nature, and low in cost are required. In this sense iron oxide is ideal for next generation anode materials. NP of γ-Fe_2O_3 are successfully prepared via facile hydrolysis of iron iodide complex precursor with following oxidation under mild conditions. Electrodes of γ-Fe_2O_3 NPs initially deliver capacities of 1100 mAh/g and increase by up to 300 mAh/g by following an activation step of the electrodes [2].

The electrodes produced from obtained in reducing media MnO_2-nanostructures were tested as electrodes of lithium ion batteries delivering initial discharge capacities of 968 mAh/g for anode (0 to 2.0 V) and 317 mAh/g for cathode (1.5 to 3.5 V) at 20 mA/g current density. At constant current of 100 mA/g, stable cycling of anode achieving 660 mAh/g and 145 mAh/g for cathode after 200 cycles is recorded. Post diagnostic analysis of cycled electrodes confirmed the electrode materials stability and structural properties [3].

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Lyotropic liquid crystals colloids as a new van der Waals heterostructures

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The integration of carbonaceous nanoparticles: fullerenes (0D), carbon nanotubes (1D), graphene nanoplatelets (2D) to a wide class of ultra-modern two-dimensional layered materials (2DLMs) like graphite, molybdenum sulfide, boron nitride have been provided a significant impulse to interdisciplinary research on the interface of physics, chemistry and engineering.

Generally 2DLMs consist of strongly bound atoms in the layer but are weakly bonded to adjacent layers or individual nanoparticles through van der Waals (vdW) interaction (also often in such of kind areas of materials science we may see this term as “vdW integration”). In other words vdW integration consists "blocks" are physically assembled together through weak vdW interactions. As result such of method offers creating new of an alternative low-energy material-integration approach.

This assembly method allows to implement isolation, mixing and combining very different atomic layers to create unique structures, as well as known heterostructures. Combining of new properties in such structures with different layers of metals, semiconductors or insulators is a promising basis for the construction of vdW heterostructures with new electronic, optical or magnetic properties [1].

In this work the first step towards the creation of mixed-dimensional vdW heterostructures as well as studying of their morphology at the molecular level was proposed. In particular, a stable aqueous lyotropic liquid crystals–carbon nanotubes composite was obtained on the basis of multiwalled CNTs and moreover we have been studied graphene oxide films adsorbed on an atomic-smooth surface of high-oriented pyrolytic graphite. Obtained results are promising for future steps of mixed-dimensional vdW heterostructures development.

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Interfacial behavior of water bound to lignin particles

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The conversion of lignin, one of three main biopolymers together with cellulose and hemicellulose in the biomass, in to value-added products is of importance from a practical point of view. Technical lignins are generated as by-products in pulp and paper manufacturing and in biomass pre-treatment processes. The structure and properties of the lignins vary depending on the wood precursors and industrial processes used to prepare final lignins, and some of these materials are water-soluble. Lignin possesses structural features that make it a promising starting material for chemical modifications, which can lead to the preparation of valuable polymeric materials. Lignins have phenolic hydroxyl groups and aliphatic hydroxyl groups at the C-α and C-γ positions on the side chains, which can be used for chemical modifications to increase the range of lignin applications. The proportion between the number of phenolic and aliphatic OH-groups in the lignin macromolecules varies depending on the isolation process. Phenolic hydroxyls as the most reactive functionalities can significantly affect the chemical reactivity of the lignin material.

In this work, a water-soluble lignin was studied upon interactions with water in different dispersion media (air, chloroform alone and with addition of trifluoroacetic acid F_3COOD, TFAA) using low-temperature ^1H NMR spectroscopy applied to static samples to study only a mobile phase of bound water at $T < 273$ K. The temperature range of 200-290 K used allows to analyze the behavior of water differently interacting with lignin macromolecules. The spectra show the presence of water clusters and domains of various sizes (strongly, SAW and weakly, WAW associated waters) and frozen at different temperatures (strongly and weakly bound waters). Interaction of water with polar functionalities of lignin results in a downfield shift of the signals of SAW. SBW is a poor solvent even for TFAA. SAW and WAW are observed even at 210 K due to strong interaction with polar functionalities of lignin and confined space effects. The obtained results allow one a deeper insight into a problem of interactions of lignin molecules with various environment that is of importance for practical applications of the materials.

Symmetry properties of pulsating ratchets

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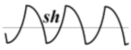
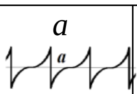
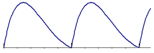
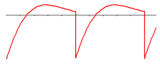
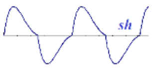
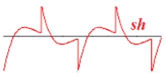
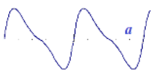
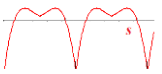
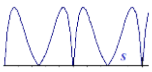
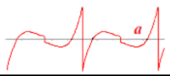
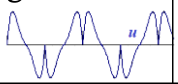
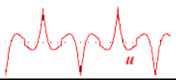
Symmetry properties play a significant role in prohibition/permission of unidirectional motion of nanoscaled objects, e.g. ratchets [1]. The Table contains symmetry properties of pulsating ratchets with multiplicative structure of nanoparticle potential energy, $U(x,t)=w(x)\sigma(t)$, and a force corresponding to it, $F(x,t)=g(x)\sigma(t)$, $g(x)=-dw(x)/dx$. There is a subtle connection between the ratchet-effect and symmetries (*s*, *a*, *sh*, *u*) of the multipliers in $F(x,t)$.

Table. Symmetry properties of pulsating ratchets

x-symmetries		t-symmetries ($\sigma(t)$)				
$w(x)$	$g(x)$	nonsymm 	*sh* 	*s* 	*a* 	*u* 
nonsymm 	nonsymm 		even	odd (o-d)	0 (o-d)	even 0 (o-d)
sh 	*sh* 	even	even	even 0 (o-d)	even 0 (o-d)	even 0 (o-d)
A 	*s* 	odd	0	odd	odd 0 (o-d)	0
s 	*a* 	0	0	0	0	0
U 	*u* 	0	0	0	0	0

The information in the cells are as follows: “0”, “even”, and “odd” mean the absence of the ratchet-effect, evenness and oddness of the functional $v\{F(x,t)\}$ (the average ratchet velocity); the “(o-d)” stresses that the property obtained is valid only in the overdamped regime of motion.

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An effective method for calculation of a Brownian ratchet driven by small sinusoidal perturbations of particle potential energy

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In a number of Brownian ratchet systems, nanoparticle potential energy has the form $U(x,t)=u(x)+\sigma(t)w(x)$, where $u(x)$ is a main part, and $\sigma(t)w(x)$ is its small perturbation. The choice $w(x)=w_0\sin(kx-c)$ allows one to control the average ratchet velocity, $\langle v\rangle$, by changing a phase shift, c. This fact has been found for low-energy ratchets ($\beta u(x)<<1, \beta w(x)<<1; \beta\equiv 1/k_BT$) [1]. In [2], a general analytical expression for $\langle v\rangle$ has been obtained. It is a double integral containing the quadratic form of $w(x)$, the equilibrium distribution functions $\rho^{(\pm)}(x)$ in potential $\pm u(x)$, the function $S(x,y)=\int_0^\infty dt\, g(x,y,t)K(t)$ including the retarded Green's function $g(x,y,t)$ of diffusion in $u(x)$, $K(t)$ is the second-order autocorrelation function. Finding $S(x,y)$ is the most difficult subtask here, additional difficulties are from the integration in the adiabatic region. We suggest a method reducing the complexity, based on the obtained Fourier analog for the integral representation:

$$\langle v\rangle = LJ; \quad J=-i(\beta DL)^2\sum_{pp'p_1p_2} k_{p'}k_{-p-p_1}k_{-p_2+p'}\rho^{(+)}_{p_1}\rho^{(-)}_{p_2}S_{pp'}w_{-p-p_1}w_{-p_2+p'}\,, \tag{1}$$

$$\left(\frac{\partial}{\partial t}+Dk_p^2\right)g_{pp'}(t)+\beta Dk_p\sum_{\tilde p}k_{p-\tilde p}u_{p-\tilde p}g_{\tilde p p'}(t)=-\frac{1}{L}\delta_{pp'}\delta(t)\,, \tag{2}$$

For $\sigma(t)$ describing deterministic periodic or stochastic dichotomous processes, the problem is reduced to finding the matrices $\left[A_{pp'}\pm \mathrm{i}\omega_j\delta_{pp'}\right]^{-1}$ or $\left[A_{pp'}+\Gamma\delta_{pp'}\right]^{-1}$, where $A_{pp'}$ are determined by the components u_p; ω_j and Γ is the frequency of Fourier component σ_j and the inverse correlation time for stochastic dichotomous $\sigma(t)$, respectively. The proposed method significantly optimizes the model and is used for calculation of $\langle v\rangle$ with different $u(x)$, $w(x)$ and $\sigma(t)$.

This work has been partially supported by Belarusian Republican Foundation for Fundamental Research (Grant No. Ф18Р-022).

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Gating mechanism as a Brownian ratchet

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A number of systems, both biological and artificial, can demonstrate the ratchet effect, the rectification of unbiased nonequilibrium fluctuations into directed motion in systems with broken symmetry. The widest class of Brownian ratchets are those with time-dependent potential energy. Within the typology by P. Reimann, potential energy of a nanoparticle in such systems can be represented as $U(x,t) = V[x, f(t)] - F(t)x$ with $V[x, f(t)] = \; = V[x+L, f(t)]$ (L is a period) [1]. The two most special cases here are tilted and pulsating ratchets with $f(t) = 0$ and $F(t) = 0$, respectively. Having a lot in common in description and operation, they are fundamentally different in frequency dependence of the average particle velocity [2], sensitivity to cusp points in dependence U on x [3] as well as to parameters of spatial and temporal asymmetry of a potential profile (see, e.g., [4] for high-temperature stochastic ratchets). There are more subtle mechanisms for emergence of the ratchet effect within the class $U(x,t) = V[x, f(t)] - F(t)x$, in particular, the so-called “gating mechanism”, in which synchronous fluctuations of a uniform force $F(t)$ and a potential $V[x, f(t)]$ can rectify nanoparticle motion even for spatially symmetric potentials and $\langle F(t) \rangle = 0$ (see [4] on the experimental realization of such a scheme).

We present results which expand the consideration of [4], the authors of which analyzed a charged nanoparticle in near-surface viscous medium, moving in stationary periodic potential $V(x,z)$ of the substrate and alternating field of a fluctuating external force $\vec{F}(F_x, F_z)$ of a fixed direction. We expand the model by introducing an asymmetric potential $V(z,x) = V_m(z)\left[\sin(2\pi x)/L + 1/4\sin(4\pi x)\right]$ of the substrate (instead of its cosine dependence on x), and by considering effects induced by the direction of the force $F(t)$. In particular, the choice of harmonic force fluctuations with time (for example, the action of an external electric field): $F_z(t) = F_{0z}\cos(\omega t)$ and $F_x(t) = F_{0x}\cos(\omega t)$ with $F_{0x} = F_0\cos\varphi$ and $F_{0z} = F_0\sin\varphi$ (φ is the angle between the force and x-axis), allowed us, within a fairly simple model (yet treated only numerically), to study effects of competition between the asymmetry of the potential and the angle φ in ratchet motion.

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Porous coatings and structures for the intensification of boiling processes on metallic heat-stressed surfaces

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The development and design of efficient two-phase heat transfer devices, which in the technology are called thermal pipes and thermosiphones, require the creation of effective metal porous materials. Such materials, depending on their thickness, may be coatings or structures. These materials were developed and created at the Institute of Materials Science of the NAS of Ukraine. The authors partially investigated the influence of a number of porous materials properties on the processes of two-phase heat exchange during boiling on metal porous surfaces.

Prolonged experimental studies of boiling water, ethanol and acetone processes on metal heat-stressed surfaces were performed under conditions typical for the operation of thermosyphons and heat pipes. The obtained results have shown that the coefficients of heat transfer α [$Wt/m^2 \cdot K$] describing the intensity of the two-phase heat transfer, depending on the physical and technical properties of the coatings and structures, can be up to 10 times greater for water compared with smooth metal surfaces. When boiling acetone and ethanol, these factors can be up to 15 times larger.

The thermal conductivity of porous metallic coatings and structures most strongly affects the coefficients of heat transfer increase. Factors such as the porosity and thickness of materials and coatings, as well as their average pore size, also affect the intensity of boiling processes. The conditions of movement of liquids in their free movement and capillary transport also have a certain influence on the intensity of boiling processes.

The authors summarized the results of the experimental studies with empirical formulas. Obtained formulas allow appropriate engineering calculations required for highly efficient heat exchange devices designing.

The influence of titanum dioxide modification with sulfur and carbon on its physico-chemical and photocatalytic properties

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Recently, modification of titania with non-metal dopants is widely used in various laboratories in order to enhance photoactivity of this popular photocatalyst and, moreover, to shift its activity into the visible range of the spectrum. Thus, this work aims at the obtaining of titanium dioxide modifications and studying their physicochemical and photocatalytic properties.

Nanocomposites were obtained by thermal hydrolysis of titanium ethylate or butylate with additions of thiourea and carbon. The samples were marked as C/TiO_2 (carbon content was varied), S/TiO_2 (sulfur content was varied) and $C/S/TiO_2$ (sulfur content was varied). XRD, SEM, TEM, BET, UV-Vis, and IR spectroscopy were used to characterize properties of the powders obtained.

All the powders were highly crystalized. Pure titanium dioxide sample was characterized by anatase and rutile phases. Samples modified with sulfur and both with sulfur and carbon were also characterized by anatase and rutile phases, whereas samples modified with carbon showed only anatase phase. Rutile phase was characteristic for the samples with high sulfur content. Brookite peaks were not observed at all.

The size of nanocomposites is decreased under modification. Thus, C/TiO_2 had size of 14–16 nm, S/TiO_2 9–10 nm, $C/S/TiO_2$ 6–9 nm.

Analysis of nitrogen adsorption–desorption isotherms for the synthesized nanocomposites showed the presence of a hysteresis loop which is the evidence for mesoporous structure of the powders.

All the modifications led to bathochromic shift as compared to pure TiO_2 photocatalyst, whereas the band gap width narrowed.

Photocatalytic activity of the composites was studied in the model reaction of destruction of dye safranin T in aqueous solutions under UV and visible irradiation. Nanocomposites were photocatalytically active in the destruction of this dye both under UV and visible light irradiation, in contrast with pure titanium dioxide, which acts as photocatalyst only under UV irradiation and might be used in environmental photocatalysis for industrial waste purification of various organic impurities, in particular, dyes that are stable in the environment. Thus, modification of this photocatalyst by non-metals can provide increasing of sensibility at longer wavelengths.

Synthesis of magnetosensitive nanocomposites with carbon surface

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Carbon sorption materials are widely used to solve various problems in engineering, biotechnology, medicine, environmental protection, *etc*.

The aim of this work is to synthesize new magnetosensitive nanostructures with single-domain magnetite-based carbon surface and research their properties.

The carbonization of the surface was realized with organic substance – reagent grade glucose.

To determine the optimal conditions of the carbonization of the magnetite surface was investigated the influence of glucose concentration, pressure, temperature and time of carbonization, the specific surface and methylene blue (MB) adsorption characteristics.

Table. Characteristics of MB adsorption on the Fe_3O_4/C nanocomposite

Conditions of synthesis	*A*, mg/g	*R*, %	Conditions of synthesis	*A*, mg/g	*R*, %
Influence of glucose (gl.) concentration			Influence of pressure		
0.15 g of gl./1 g Fe_3O_4, 5 atm, 180 °C	0.65	37	0.33 g of gl./1 g Fe_3O_4 1 atm, 180 °C	1.4	68
0.33 g of gl./1 g Fe_3O_4, 5 atm, 180 °C	2.9	100	0.33 g of gl./1 g Fe_3O_4, 2,5 atm, 180 °C	2.2	74
0.45 g of gl./1 g Fe_3O_4, 5 atm, 180 °C	3.2	100	0.33 g of gl./1 g Fe_3O_4, 5 atm, 180 °C	2.9	100
0.65 g of gl./1 g Fe_3O_4, 5 atm, 180 °C	2.3	74	0.33 g of gl./1г Fe_3O_4, 7,5 atm, 180 °C	2.0	87
Influense of temperature and time of carbonization					
0.33 g of gl./1 g Fe_3O_4, 5 atm, 180 °C, 6 h	2.9	100	0.33 g of gl./1 g Fe_3O_4, 5 atm, 300 °C, 3 h	1.1	70

The optimal conditions of the carbonization of magnetite is: glucose concentration is 0.3-0.5 g per 1 g of magnetite, $P = 5$ atm, $T = 180°C$ during 6 h.

The synthesized nanocomposite is prospective for creation of new magnetosensitive sorbents for medical-biological, technical and ecological purposes.

Properties of active charcoal from waste of smoking industry

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The purpose of our work was to evaluate the properties of potential sorbents, obtained from technological waste of the food industry. They must be suitable for cleaning various environments, including water-alcohol raw materials.

Activated carbon (AB) with a high yield, developed specific surface (mainly with micropores) was obtained by the method of alkaline activation of pyrolyzed wood waste from smoking industry - carbonized chips (CC). Their high sorption capacity towards phenol, lead ions and dye - methylene blue (MB) - were determined [1] (Table).

Table. Conditions of ACs obtaining and their characteristics

Index	Units	Title of index	AC from lignite		AC from CC	
Activation temperature , K			1073		1073	
State of activating agent, KOH			solid		50%-solution	
Raw material / agent, kg / kg			1:0.5		1:1	
Y	%	Yield	39.0		70.4	
S_{BET}	m^2/g	Specific surface area	890		777	
V_{Σ}	cm^3/g	Total porous volume:	0.58	100%	0.42	100%
V_{mi}	cm^3/g	micropores	0.32	55.2	0.30	70.3
V_{1nm}	cm^3/g	subnanopores	0.23	39.7	0.25	59.2
A_{Φ}	mg/g	Sorption of phenol	120		200	
A_{Pb}	mmol/g	Sorption of Pb^{2+}	–		0.7	
$A_{МБ}$	mg/g	Sorption of MB	92		150	

The best result on the quality of the vodka according to the results of the findings of 3 professional tasters was set for AC from wood waste of smoking production, activated with KOH. Estimates of the vodka purified by it were 9.68-9.70 against 9.4-9.6 for the initial sorting and after purification with AC, obtained by activating CC with orthophosphoric acid.

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One-sided broadening of the frequency dependence of ratchet velocity

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In the theory of Brownian motors (ratchets), controlled by a dichotomous process with average lifetimes of states τ_+ and τ_-, the adiabatic approximation is valid when each of these times is much longer than the diffusion time $\tau_D = L^2 / D$ over a spatial period L of potential energy (D is the diffusion coefficient). Therefore, within this approximation, the average ratchet velocity v does not depend on the time asymmetry parameter $\varepsilon = (\tau_+ - \tau_-)/(\tau_+ + \tau_-)$ and is inversely proportional only to the sum of the times τ_+ and τ_-. It is known, that the dependence of the velocity v on the frequency of potential energy fluctuations, determined by the dimensionless parameter $\xi = (L/2\pi)^2 / D\tau$, $\tau = \tau_+ + \tau_-$, is characterized by a bell-shaped form [1]. To compare these dependences with those obtained experimentally, it is convenient to characterize them by the position of maximum ξ_m and the distribution width at half-height w. It can be expected that with a change in the parameter ε these distributions will demonstrate unilateral widening, since a left (low-frequency) wing of a distribution, which corresponds to the adiabatic regime, does not depend on ε. To verify this assumption, we used analytical expressions for the average velocity of a high-temperature ratchet with a potential profile of a sum of two sinusoids [1]. The results are shown in the Fig., which proves our assumption.

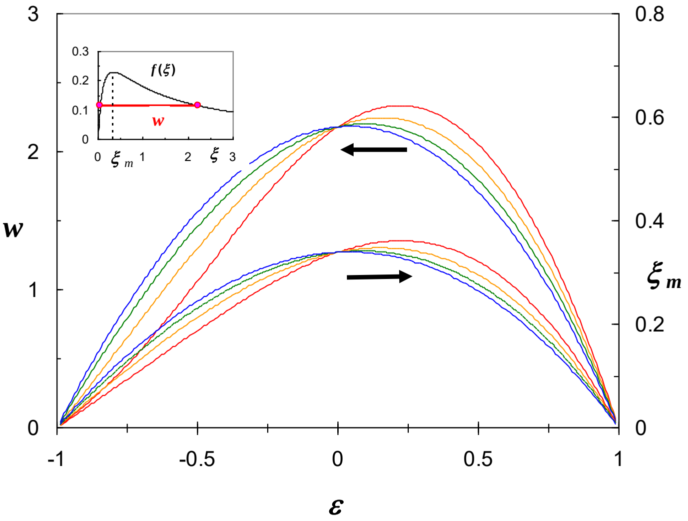

Fig. Dependencies of the distribution width at half-height w (the insert illustrates the definition of w) and of the maximum position ξ_m on the asymmetry parameter ε (*left and right axis, respectively*). Each family includes curves calculated for different ratios of potential energies in two states of the dichotomous process

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Composite nanostructures based on crystalline graphitic carbon nitride for efficient photocatalytic hydrogen production under visible light

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The photocatalytic properties of composite nanostructures based on crystalline graphitic carbon nitride (CGCN) [1], modified by metal nanoparticles, in the process of molecular hydrogen production from water-alcohol mixtures under visible light have been studied. Metal nanoparticles were deposited by *in situ* photocatalytic reduction from solutions of the corresponding salts. It is shown that the dependence of the photocatalytic H_2 emission rate on the metal content in the obtained nanocomposites has the shape of a curve with a maximum (Fig., *a*), and their activity significantly depends on the nature of the metal in the composite and increases in the row CGCN/Au(1%) < CGCN/Pd(0.4%) < CGCN/Pt(0.5%) (Fig., *b*) at the effective metal content.

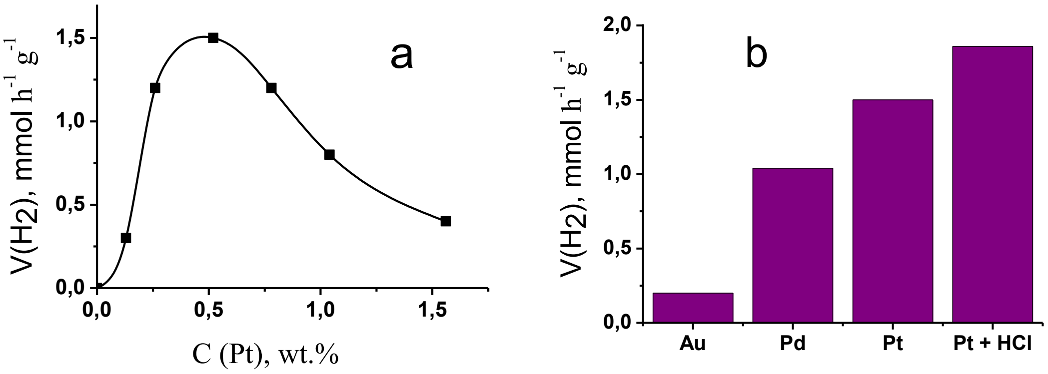

Fig. The dependence of the activity CGCN/Me composites in photocatalytic hydrogen production under visible light on the platinum content (*a*) and the nature of the metal (*b*)

Using the CGCN/Pt nanocomposite photocatalytic system as an example, it was found that the small addition of acid (0.1 mol/L HCl) leads to the increase of the H_2 formation rate (Fig., *b*), and effective metal content in the composite can be reduced from 0.5 to 0.25 wt.%. The highest rate of hydrogen production achieved using CGCN/Pt was 1.9 mmol h^{-1} g^{-1}.

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Solution combustion synthesis of bimetallic and metal-ceramic nanomaterials

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The aim of this work is to investigate the possibility of bimetallic nanopowders synthesis by solution combustion synthesis in normal air atmosphere without additional post reduction. The following materials were used in the experiments: copper nitrate – $Cu(NO_3)_2{\cdot}3H_2O$, "analytical grade" GOST 4163-78; cobalt nitrate – $Co(NO_3)_2{\cdot}6H_2O$, "analytical grade" GOST 4528-78; nickel nitrate – $Ni(NO_3)_2{\cdot}6H_2O$, "analytical grade" GOST 4055-78; citric acid hydrate – $C_6H_8O_7{\cdot}H_2O$, "analytical grade" GOST 908-2004; iron(III) nitrate – $Fe(NO_3)_2{\cdot}9H_2O$, "analytical grade" TU 6-09-02-553-96; urea – CH_4N_2O, "analytical grade" GOST 6691-77 and hexamethylenetetramine – $C_6H_{12}N_4$, "analytical grade" GOST 1381-73.

It was revealed that the optimal reducing agent for obtaining bimetallic ultrafine materials from organic-salt mixtures, including copper and nickel nitrates, was hexamethylenetetramine at fuel-to-oxidizer ratio $\varphi = 1.75$, pH=6–7. The resulting powder consists of metallic copper and a solid solution of $Cu_{0.51}Ni_{0.49}$ (a = 3.5701 Å). Coherent scattering region (CSR) – 50–60 nm. Metal-ceramic materials, constituting metals and their oxides, were synthesized in the following organic-salt systems: $Cu(NO_3)_2$ – $Ni(NO_3)_2$ – fuel (φ – 1.25 and 1.75); $Cu(NO_3)_2$ – $Co(NO_3)_2$ – fuel (φ – 1.5 and 2.0). CSR - 50–60 nm. In addition, the possibility of obtaining of metallic powder consisting of metallic copper and solid solution of copper, cobalt and nickel (a = 3.740 Å) in the $Cu(NO_3)_2$ – $Co(NO_3)_2$ – $Ni(NO_3)_2$ – $C_6H_{12}N_4$ system with $\varphi = 4.0$ and pH = 6–7. CSR - 40–50 nm. Material consisting of copper ferrite $CuFeO_4$ and tenorite CuO was obtained in the $Cu(NO_3)_2$ – $Fe(NO_3)_3$ – $C_6H_8O_7$ system at pH = 6–7 and φ=2.0, which can be used to produce middle temperature next-generation catalysts for converting CO.

The results of research can be used in the production of automotive catalytic neutralizers of exhaust gases, in oil refining, chemical industry, nanoelectronics, optics, photochemistry, medicine and other fields.

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Thermophysical properties of epoxy composites with modified nanosilica particles

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Thermal destruction for composites of epoxy resin "Epoxy 520" with modified nanosilica particles for loading of $0 < C \leq 5\%$ have been investigated. As fillers, the nanoparticles of silica A-300, densed silica A-300 D, obtained by means of mechanochemical treatment of A-300 in a ball mill, silica A-300 D modified with iodide silver particles AgI and AgI nanoparticles were used. Mechanochemical treatment results in a decrease of the specific surface for the pristine silica from S ~ 285 m^2/g to 260 m^2/g for A-300 D. Coating of A-300 D with AgI particles lowers S to 240 m^2/g. Phase transition to the conductive state at temperatures $T \geq 90$ ^{o}C occurs at the iodide silver particles.

Investigations were performed by method of thermodesorption mass spectrometry. Desorption curves for CO_2 fragment with m/z 44 (m is a fragment mass, z is a fragment charge) reflect the loading effect with modified particles on thermodestruction of composites (Fig.).

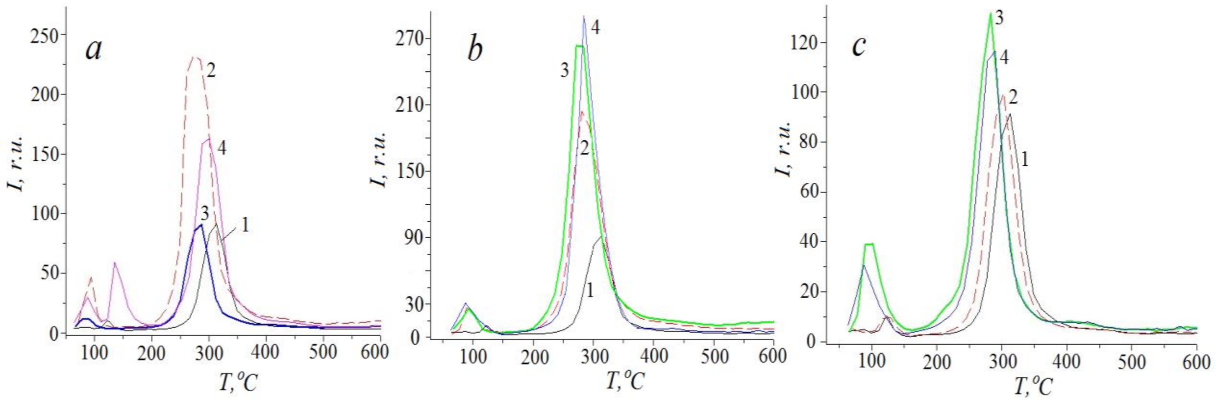

Fig. Thermal desorption curves of CO_2 fragment for epoxy resin filled with A-300 D (*a*), AgI (*b*), A-300 D + AgI (*c*) upon concentrations of 0 (*1*), 1 (*2*), 3 (*3*) and 5% (*4*)

It is shown that filling with densed A-300 D particles weakly increases the epoxy composite thermal stability. The loading of iodide silver particles slightly decreases the composite thermal stability. Bright rise of the thermal stability is found in the composites with A-300 D particles modified with AgI. Thus, the hybrid epoxy composites with particles A-300 D coated with AgI have the maximal thermal stability.

Electrophysical properties of composites based on the epoxy resin and carbon nanotubes

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Nanocomposites (NC) on the basis of carbon nanostructures were introduced in nanoelectronics, optics, instrumentation and material science. The unique structure of carbon nanotubes, their high values of strength, electric and thermal conductivity in the axial direction make it possible to create NC with high performance characteristics. For the best chemical or physico-mechanical characteristics (high impact strength, low combustibility, *etc*.) to the components of conductive NC fillers of different nature, more often inorganic, are added.

The purpose of the work is to establish the laws of the electrophysical properties NC, depending on the content of the multi-wall nanotubes (MWNT) and the nature of the surface of the dielectric components.

On the basis of the epoxy resin (ER) four series of specimens were made: MWNT-vermiculite-ER, MWNT-perlite-ER and two such series with the addition of sand. The content of the MWNT was varied from 0.1 to 2% by weight, the epoxy resin was used as the binding agent.

Electrophysical characteristics – dielectric permittivity ε' and specific electrical conductivity σ were measured at low frequencies of 0.1, 1 and 10 kHz by two-contact method with the help of the immittance meter E7-14.

The values of the components of the complex permittivity in the absence of nanotubes are the same for all systems under study. If the content of nanotubes is greater than 1%, that is above the percolation threshold, then in each system the growth ε' and ε'' is due to the formation of a continuous CNT cluster. The corresponding electrophysical properties of the system containing vermiculite are higher in samples without sand and smaller in samples with sand. For systems without sand, the values of ε' and ε'' for vermiculite are higher by 25 and 60%, respectively, than perlite. In systems containing sand, the corresponding values for perlite are higher by 25 and 30%, respectively. The presence of sand for perlite systems increases the value of ε' by 1.5 times, which emphasizes its structural effect.

Thus, the electrophysical characteristics of the investigated systems with the content of multi-wall nanotubes essentially depend on the nature of the surface of the dielectric components of composite systems. Changing the content of such dielectric ingredients allows us to expand the functionality of composites used for shielding from electromagnetic fields.

Change of qualitative composition of the phenolic compounds at cultural medium of the *Azotobacter vinelandii* IMV B-7076 at their cultivation with palygorskite nanoparticles

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Palygorskite clays are natural nanostructured material with unique properties and wide possibilities of use in modern technologies, including the creation of the latest microbial biotechnologies.

The microorganisms interact with natural nanomaterials, a layer of highly dispersed particles forms on the cell surface. This can have a significant impact on the properties of the surface of bacterial cells, their functional activity, in particular the synthesis of metabolites, antioxidants of phenolic nature. The latter has an important role in maintaining the homeostasis of cells.

Using a GC/MS analysis of the methanol extract of the culture medium *Azotobacter vinelandii* IMV B-7076, a number of compounds of phenolic nature were found: 1,2-benzenediol (catechol), hydroquinone, and 2,3-dihydroxy-benzoic acid. The cultivation of this strain with 0.05 to 0.5 g/L of palygorskite nanoparticles for 48 hours, only 1,2-benzenediol was identified among the phenolic metabolites. Perhaps the absence of second other compounds, based on their chemical structure, is due to the adsorption of the latter on the nanomaterial under study. Thus, the symmetric hydroquinone molecule, due to the presence of 2-nd hydroxyl groups, can easily interact with the surface of clay mineral [1]. The high adsorption capacity of 2,3-dihydroxybenzoic acid is due to the location of the OH group in the meta-position. The hydroxyl groups of 1,2-benzenediol in the ortho-position most likely form a chelate structure with one of the active centers of the palygorskite through two free hydroxyls on its surface. However, these superficial groups of clay minerals are not always available, which respectively affects the reduction of the sorption activity of the catechol [2, 3].

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The study of the malonic acid adsorption at the hydroxyapatite/aqueous electrolyte interface

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The organic-inorganic interface is of importance since it provides the active sites for biological control in biomineralizations. An important but largely unresolved issue is the way in which nature controls the nucleation, growth, and morphology of inorganic crystallites and the function of biomolecules (such as amino acids and proteins) in these reactions [1].

Surface properties of hydroxyapatite were studied before and after adsorption using X-ray diffraction (XRD), adsorption-desorption of nitrogen (ASAP), PCS (photon correlation spectroscopy), FTIR. Physicochemical properties of hydroxyapatite [$Ca_{10}(OH)_2(PO_4)_6$] surface were studied by means of potentiometric titration and electrophoretic measurements. The surface charge density and zeta potential was measured for the basic electrolyte concentrations (0.001 mol/dm^3) as a function of pH and concentration of the malonic acid ranged from 0.001 to 0.000001 mol/dm^3.

The specific adsorption of malonic acid ions at the hydroxyapatite interface was investigated by means of the radioisotope method (^{14}C) as a function of malonic acid ions concentration, NaCl concentration and pH. Physical properties of the powder were characterized by XRD and FTIR. Physicochemical properties characterizing the electrical double layer of the hydroxyapatite/NaCl solution interface were determined. The zeta potential and the adsorption of malonic acid molecules were studied as a function of pH. The point of zero charge and the isoelectric point of samples were determined: its values are as follows pHpzc=7 and $pH_{IEP}<4$. Two phenomena are responsible for malonic acid adsorption: phosphate group replacement at the hydroxyapatite surface by malonic acid simultaneous to intraspherical complexes formation. The malonic acids adsorbed on the HAP faces negative carboxylate groups occupied vacant P or OH sites precisely and formed an ordered adsorption layer.

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Study of the grain size and zeta potential of selected clays alone and in the blends with nanosilica A-300

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Clay is defined as naturally occurring material composed mainly of fine-grained minerals. Clay is generally plastic at appropriate water content, and it is hardened as dried or fired. Clay usually contains phyllosilicates; however, clay might contain other materials which can affect the properties [1]. Clay associated phases may include organic matter and materials which do not impart the plasticity. Geologists and soil scientists use term “clay” at the particle sizes less than 2 μm, as well sedimentologists - 4 μm and colloid chemists - 1 μm. Clay minerals can be negatively charged (most of clay minerals), positively charged (e.g. layered double hydroxides, LDH) or uncharged (often found, e.g. talc and pyrophyllite). All clay minerals are porous with pores of varied sizes and shapes. Arrangement of the layers and assemblies of particles leads to different morphologies (e.g. plates, tubules, laths, and fibres). Depending on the clay structure formed during mineral formation, different physical, chemical and mechanical properties could be exhibited.

The particle sizes and zeta potential of the aqueous suspensions of clay samples (kaolinite, china clay, white-blue clay, white clay and nanosilica as well white-blue and silica composites, in the majority of the selected systems) were measured using a Zetasizer Nano ZS90 (Malvern). The results of the zeta potential measurements shows that pH_{IEP} was below 2. The total surface charge at clay/electrolyte interface results the isomorphic substitution of Si^{+4} and Al^{+3}ions in the phyllosilicate lattice forming structural charge and reaction of surface hydroxyl groups with the electrolyte ions creating net adsorbed proton charge density [2]. Because isomorphic substitution lead to negatively charge that dominate over charge the surface of clays at pH>2 is negatively charged. Dispersed particles of clays undergo coagulation the result in the delamination of the samples.

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Decolorization of malachite green on the mesoporous SiO_2/TiO_2 films: effect of Ag nanoparticles deposition

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The adsorption and photodegradation processes of aqueous solution of Malachite Green (MG) over SiO_2, TiO_2 and SiO_2/TiO_2 films as well as the films modified with Ag nanoparticles were investigated *in situ* by UV-Vis spectroscopy and LDI mass-spectrometric methods.

The transparent porous SiO_2, TiO_2 and SiO_2/TiO_2 thin films were synthesized via low-temperature sol-gel route in the presence of template agents used to create the developed porosity and high surface area. Ag-modified films have been prepared via consequent photo- and thermoreduction of Ag^+ ions added to the precursor as $AgNO_3$ (10^{-3} M) by UV-irradiation of deposited films followed by thermal treatment at 500°C. From bright yellow color and the intensive broad surface plasmon resonance band (SPR) (λ_{max}=450 nm) in absorption spectra of $SiO_2/TiO_2/Ag$ films, we can conclude that the broad size distribution of Ag nanoparticles occurs.

MG adsorption on the surface of SiO_2 and TiO_2 films is reversible: the dye molecules can be easily desorbed from the films' surface. However, they are not able to leached from TiO_2/SiO_2 surface that can be interpreted in terms of protonation through basic N-dimethylamino groups by acidic OH groups of mixed oxide surface as observed by us early for 9-aminoacridine on silica surface [1]. Photobleaching of MG in aqueous solution in the presence of the investigated films proceeds via discoloration of MG under dark condition (connected with the dye leuco-form formation as the result of proton transfer processes on the semiconductor surfaces), color recovering due to photodesorption process under UV irradiation and efficient photodegradation of MG. Addition of Ag nanoparticles into mesoporous TiO_2 films leads to enhancing and accelerating of this process. The most effective photooxidative degradation of MG occurs on silica-titania films and films modified with Ag nanoparticles. LDI mass-spectrum of dye molecules adsorbed on mesoporous SiO_2 and TiO_2/SiO_2 films varies from complete dominance of cation peak to more complicated proportions where, in addition to unconditionally prevailing peak $[M^{+1}]^+$, the noticeable intensive peaks ($M^{+\cdot}$, $[M^{+2}]^+$) might be present. Ag peaks (*m/z* 107, 216 and 323) do not interfere with analyzed peaks.

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ZnAl layered double hydroxides for absorption and photocatalytic removal of tetracycline antibiotics

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The preparation of the multifunctional assembly in which the different components may act in synergism is an approach that allows to obtain materials combining several properties. Special attention is now paid to the layered double hydroxides (LDH) because of their flexibility of the chemical composition of the metal hydroxide-based layers and the interlayer anions. LDH consist of stacks of positively charged mixed metal hydroxide layers that require the presence of interlayer anions to maintain overall charge neutrality.

The potential sorbents capacity of LDH for organic molecules makes these materials attractive as possible filters for water containing antibiotics contaminants. Pharmaceutical antibiotics have been applied worldwide in human therapy and the farming industry. Thus, antibiotics (especially tetracycline antibiotics) have attracted many people's attention recently. Tetracycline (TC) has been considered to be a class of potential pollutants [1]. Most TC antibiotics enter the environment through municipal effluent, sewage sludge, solid wastes, and manure applications.

Recently, LDH have been intensively investigated as promising heterogeneous photocatalysts because of their intrinsic photo-response characteristics. LDH as photocatalysts showed large energy-conversion efficiency as a result of the high dispersion of active species in a layered matrix, which facilitates the charge separation. Mixed oxides with semiconducting properties are obtained by calcination of appropriate transition metal-containing LDH.

The results of the search of optimal conditions for obtaining of Zn-Al LDH with the maximum of adsorptive capacity and photocatalytic activity for the removal of the antibiotic TC will be presented. The starting materials for the investigation were Zn-Al LDH with Zn:Al ratios 2:1, 3:1, and 4:1 that were treated at the different temperature. The crystalline structure, textural and morphological properties, and bandgap edges were studied.

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Development of methods for applying titanium coatings on the elements of friction nodes of joint prostheses

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Treatment of patients with various diseases and post-traumatic injuries of the joints is currently one of the most significant medical and biological problems. Nowadays, a number of materials have been developed in Ukraine for the manufacture of friction unit components of joint prostheses, namely, artificially grown sapphire, the chemical purity of which is much higher than other materials used for these purposes. To ensure good fixation of the joint prosthesis components, a nanostructured titanium coating is applied to the liner of the acetabular cup made of artificially grown sapphire (Fig.). For this was applied vacuum arc coating technology. The sapphire component of the implant is a dielectric, in connection with this, the cleaning and heating of the sapphire surface in the gas plasma of a vacuum-arc discharge on a floating potential was applied. After sapphire insert heating to a temperature of 300 °C, a titanium coating (50–70 μm) was applied with a maximum content of the droplet phase. Drops of Ti with sizes from 10 nm to 10 μm create a very developed rough surface, which provides reliable fixation.

Fig. Photos of the sapphire insert surface with a titanium coating at different magnifications

The use of materials irradiation will allow for increased biocompatibility of implants with the tissues of a living organism, which in turn will reduce the time required for the restoration of patients' performance and reduce the risks of possible rejections.

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Fabrication of improved rare-earth (Eu) complexes-embedded aminosilica microparticles

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Lanthanides possessing unique spectral-luminescent properties are integrants of various functional materials used in display and transmission devices, optical amplifiers, or light sources. Among others, europium is used for luminescent sensing of the structure of various natural and synthetic objects. Inorganic matrix contributes to eliminating radiation-free energy losses and increasing the luminescence signal of Eu(III). This research is focused on the preparation of amine-containing silica microparticles with embedded Eu(III) complexes with different coordination surrounding of Eu achieved by varying the nature of the surface layer of the particles. The syntheses of aminosilica microparticles were based on the sol gel approach, while Eu(III) ions were adsorbed from aqueous solutions. The relevant adsorption isotherms and emission spectra are presented in Fig. We can conclude that such aminosilica could adsorb up to 1.1 mmol/g of Eu(III) ions and the intensity depends on the surface concentration of Eu(III), also all observed emission bands are due to $^5D_0$–^7F_J (J = 1, 2, 3, 4) transitions of Eu^{3+}ions.

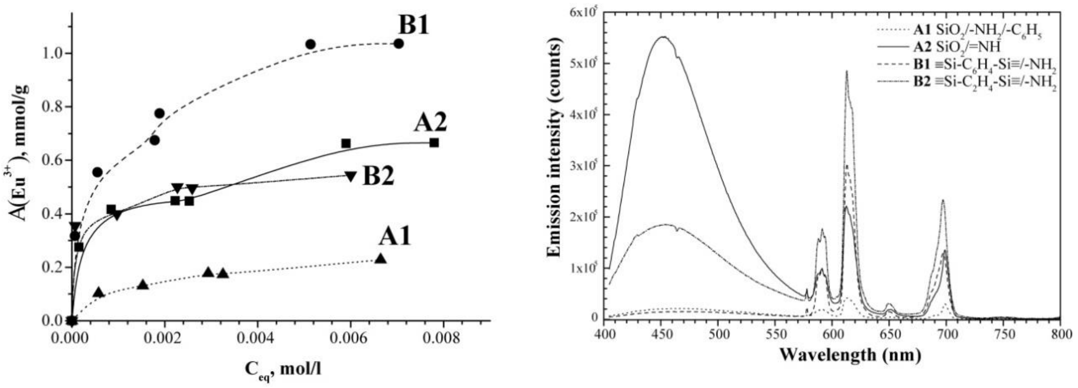

Fig. Eu(III) ions adsorption isotherms and emission spectra for the Eu(III) complexes-embedded aminosilica samples

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Investigation of drug desorption from carbon nanotubes and their chitosan composites to simulated body fluid

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Among many fields of applications of carbon nanotubes (CNT), a nano-sized drug carrier seems to be one of the most often investigated topic. Due to their large specific surface area and various possibilities of its chemical modification they seem to be perfect for nanomedicine applications [1-3].

Another material gaining more and more interest of the researchers working on nanobiomaterials is chitosan. Its main advantage is large biocompatibility and bioavailability what makes possible to deliver desired substance to the organism in safe way [4, 5] and securely deplete the carrier making no harm to body exertion system.

Combination of both materials, additionaly enriched with magnetite nanoparticles which can greatly enchance accumulation possibilities of drug loaded particles in desired place, (not to mention on their influence on sorption and desorption processes of loaded drugs) [6], may lead to invention of novel drug carrier with unique properties for tailored drug therapy.

In our investigation, we synthesized series of nanomaterials containing all three components in various combinations. The morphology of the obtained materials was investigated using STEM and XRD techniques.

Next stage of our experiment was to estimate the ability of obtained materials for controlled drug relase in *in vivo* conditions. After loading them with five model drugs, we investigated quanity and kinetics of drug release to simulated body fluid (SBF) – a mixture simulating composition of human plasma, in conditions closest to those present inside our bodies [7].

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Textural and structural characterization of carbon nanotubes/poly(dimethylsiloxane) composites

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Over past decades composites based on multi-walled carbon nanotubes (MWCNTs) and poly(dimethylsiloxane) PDMS have attracted increasing attentions due to their great potentials in wearable devices, electronic skins, human motion detection, human–machine interfaces and health monitoring.

The present study provides the textural and structural features of MWCNTs/PDMS composites. Polymer fluids of two molecular weights (PDMS-100 and PDMS-12500 with $M_w \approx 3410$ and 39500 g/mol, respectively) were adsorbed onto nanotubes surfaces in amounts of 5 – 40 wt. %. The textural properties of the samples were analyzed based on the low-temperature nitrogen adsorption/desorption. The morphology and additional structural characterization of polymer composites have been obtained using SEM studies and Raman spectroscopy. The influence of the chain length and PDMS concentration on the structure of polymer composites has been analyzed.

Three main bands are in the Raman spectra (Fig.). The ratio between the integral intensities of the G and D bands (A_G/A_D ratio as a measure of the graphitization degree) is an indicator of the crystallinity degree. It was found that the value of A_G/A_D for pure MWCNTs is greater (1.1), than for MWCNTs/PDMS composites (0.95) and indicates the higher degree of graphitization.

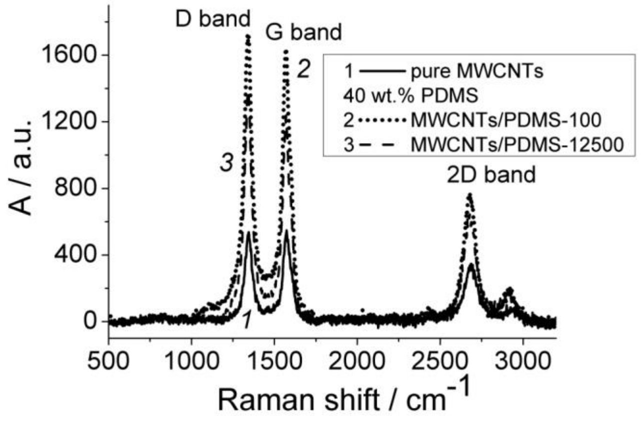

Fig. Raman spectra of pure MWCNTs (*1*) and polymer composites (*2, 3*)

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Titanium alkoxide complexes as molecular models for surface interaction between drug and sol-gel derived titania nanoparticles for drug delivery

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Titania nanoparticles are attractive mediators for drug delivery [1,2] and can be produced with fine control via sol-gel synthesis. The surface interaction between titania nanoparticles and different medical agents can be studied via complexes of pharmaceuticals. Surface chemistry can be revealed by structural studies. Here [3,4], two new coordination complexes $[Ti_4(\mu_3\text{-}O)_2(\mu_2\text{-}OEt)_2(C_9H_{16}O_3)_2(C_8H_{12}O_3)_2(C_{12}H_6Cl_3O_2)_2\cdot 4C_3H_6O]$, **1**, and $[Ti_5(\mu_3\text{-}O)_2(\mu_2\text{-}OEt)_5(\mu\text{-}OEt)_8(C_9H_{16}O_3)(C_{12}H_6Cl_3O_2)]$, **2** (Fig.) were synthesized and their structures were determined by single crystal X-ray diffraction. Triclosan coordinate to titanium atoms via phenoxide bonding. Hydrolysed compound **1** was tested against *Staphylococcus aureus* and was found to have an inhibitory effect. Thermolysis and hydrolysis of compound **1** were studied. High thermal stability of phenoxide ligands causes topotactic transformation upon calcining. The phenoxide ligands does not stabilize compound **1** against water, but hydrolyses to titania (anatase) nanoparticles with primary size of about 5 nm, as determined by transmission electron microscopy.

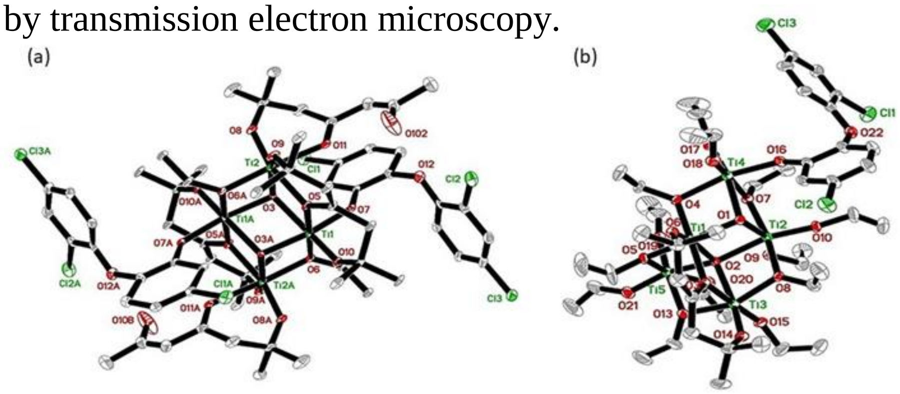

Fig. Structures of compounds **1** (*a*) and **2** (*b*). Small green is titanium, red is oxygen, grey is carbon and large green is chlorine

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Photocatalytic degradation of rhodamine B using clinoptilolite which contains cations of the transition metals

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Natural zeolites including clinoptilolite are known to be effective sorbents of many metals from aqueous solutions. In particular, the high adsorption capacity of clinoptilolite allows to use it for purification drinking and sewage water from heavy metals as well as for their preconcentration in order to quantify. Clinoptilolite itself is not a semiconductor. Therefore, it is used only as a support in photocatalytic processes as a rule.

We studied photodegradation of rhodamine B (RhB) using spent clinoptilolite after preconcentration of trace amounts of transition metals (Ag, Cu, Mn, Cr). It is known that UV-Vis spectra of synthetic zeolites have not absorption in the range of $\lambda > 300$ nm while the spectra of natural clinoptilolilte (NC) contain bands around 350 and 395 nm. These features evidently are due to impurities (iron and titanium oxides). The used natural clinoptilolite was from the deposit near the village of Sokyrnytsia (Ukraine). It contains 85–90 % of the main component and has the specific surface area, determined by water sorption, about 59 m^2/g. Besides, clinoptilolite, among other impurities, contains 0.26 wt.% of TiO_2 and 1.51 wt.% of iron oxides. As a result, NC shows some photocatalytic activity: the rate constant of RhB degradation K_d is $3.0\cdot10^{-5}$ c^{-1}. H-clinoptilolite has been obtained *via* treatment of NC with 1 M solution of HNO_3 which results in partial removal of impurity oxides. Therefore, H-form of clinoptilolite demonstrates, first of all, adsorption properties towards RhB. Additional incorporation of transition metals leads to the appearance of new bands in the spectra and some red shifts in the absorption edge towards longer wavelengths, namely to 427-447 nm. The latter corresponds to a band gap E_g = 2.90-2.77 eV. Therefore, the doping of clinoptilolite by adsorption of transition metal cations increases the photocatalytic activity by 2-3 times, although the content of these cations is, as a rule, less than 1% w/w. Thus, the value of K_d is $6.0\text{-}6.4\cdot10^{-5}$ c^{-1} for clinoptilolite doped with 0.3-0.35 % of Cu, Mn, Cr and Ag. It is interesting that silver-containing clinoptilolite causes direct degradation of RhB unlike the samples containing other metals.

Transport properties of nanographite modified with nickel and iron

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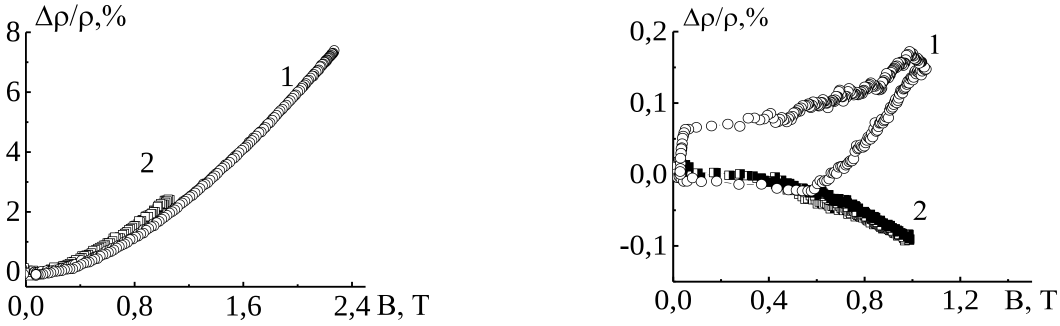
Present work is devoted to questions of creation of new nanocomposite materials based on nanocarbon particles and investigation of their electrical and magnetic conductivity. As source materials for obtaining the nanocomposites the two types of nanocarbon materials have been used. These are nanographite platelets obtained by sonication of thermoexfoliated graphite in acetone and multiwall carbon nanotubes obtained by arc-method. The modification of the nanocarbon particles has been carried out with method of reducing the metal from the water-salt solution in the stream of the mixture of gaseous helium and hydrogen. As results the nanographite platelets and carbon nanotubes with metal particles (80% mas. Ni : 20% mas Fe) on the surface have been obtained.

For investigations of transport properties bulk specimens from modified CNT and graphite nanoplatelets powder have been prepared by cold compacting with use PVA (20% mass) as binder.

Figure presents the dependences of magnetoresistance $\Delta\rho/\rho$ of modifided nanocarbon specimens at different temperatures.



a *b*

Fig. The dependences $\Delta\rho/\rho$ for modified nanographite platelets (*a*) and carbon nanotubes (*b*),
1 – T = 293 K, *2* -. T = 77 K

As it is follows from Figure for modified nanographite platelets the dependence of magnetoresistance from magnetic field is quadratic and the magnetoresistance is weekly dependent on temperature. For modified carbon nanotubes hysteresis in the $\Delta\rho/\rho(B)$ dependence at room temperature is observed, that is characteristic for systems with alternating magnetic and non-magnetic layers.

The study of microflora of active sludge in biochemical cleaning process by FTIR spectroscopy

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Among the methods used for cleaning household and industrial wastewater, biological treatment is the cheapest available, but in practice it is often the only possible one. Microorganisms of activated sludge, being in waste liquid, absorb polluting organic and inorganic substances inside the cell and subject them to biochemical transformations.

The study of the chemical structure and the degree of activity of the microflora of activated sludge will determine its application for the destruction of various types of ore and non-metallic materials used in the mining and metallurgical industries.

According to IR spectroscopy data, the chemical composition of activated sludge is represented by humic compounds, which are distributed over the entire spectrum length in the range from 500 to 4000 cm^{-1}. Phosphorus compounds, manifested in the form of vibrations of P–O, P=O, P=S, P–O–P, O–P–O bonds, are in the wavelength range from 500 to 1000 cm^{-1}. Functional nitrogen compounds distributed as KNO_3 display in the spectrum at 1000 cm^{-1}, and ammonium, amine and ammonia bonds are manifested the range of vibrations from 2400 to 3500 cm^{-1}. Potassium compounds are expressed as KNO_3 and KOH, at 1000, 1600 and 3600 cm^{-1}, respectively. The found out macronutrients are distributed in a very wide wavelength range and likely are formed a part of the composition of aromatic compounds. Heavy metals are an essential components of the mineral phases of the sludges: clay minerals, oxides and hydroxides of iron and aluminum, calcium and magnesium carbonates. During soil application, they only can be as macronutrients for their assimilation by plants.

Thus, the biological component of activated sludge takes part in the process of metal binding, i.e. microorganisms that have different functional groups on their surface. At the same time, both the organic component – protein molecules and humic-like substances – and the mineral components of sludge – silicates and aluminosilicates are involved in the process of binding metalls Exactly the property of organic matter to form chelates is related to their ability to transform inorganic compounds into a plant-digestible form.

The interaction of microflora of activated sludge with low-grade phosphorites of the central Kyzylkum

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At the present time, there is an acute problem of finding new rational ways of processing substandard phosphorites of the Central Kyzylkum region into high-quality phosphate-containing fertilizers.

The aim of this work was to study the destruction degree of the main phosphate mineral francolite (fluor-carbonate-apatite) and calcite, the ore constituents of 80-90% by microflora of activated sludge (AS) taken from the station of biochemical purification of municipal waste. Low-grade phosphorites and wastes of the Kyzylkum Phosphoritic Combinat (CPC) NMMC were used as initial materials for obtaining a new type of organic-mineral fertilizer fortified with phosphorus and AS.

IR spectra of the initial low-grade phosphate ore and after its interaction with the microflora of activated sludge showed that the absorption degree of infrared rays in the phosphate rock ranged from 0 to 14%, indicating a large amount of mineral, inorganic mass. In the interval from 1000 to 1600 cm^{-1}, the peaks remain at the zero level, due to the fact that the mineral mass of francolite does not absorb infrared radiation and does not form functional groups.

In the IR spectra of phosphate ore after interaction with the microflora of activated sludge in the range of 3200-4000 cm^{-1}, instead of the slightly sloping peaks, there are separate narrow peaks due to the transformation some functional groups in the presence of oxygen. Phosphorus compounds, which contain the following functional groups $[PO_4]^{3-}$, P-OH, P=S, P-O, P=O, O-P-O, underwent a significant functional changes. After the interaction with microorganisms of AS francolite becomes less dense, phosphorus compounds and other elements pass into a soluble form and the bandwidth narrows somewhat. Appeared under the influence of microorganisms, new functional groups have great activity, which leads to the formation of a new of mineral form.

Thus, the analysis of the IR spectra of phosphorite ore and its mixture with activated sludge in various proportions made it possible to determine the most promising composition of such a mixture to create organic fertilizer, as well as to select a special technological scheme for processing phosphate ore and sludge.

Theoretical study on the effect of carbon nanotubes on the strength of covalent bonds of nylon in a nanocomposite

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Taking nylon dimer and the model of the fragment of the outer surface of a carbon nanotube (CNT), as an example, using the method of density functional theory with functional B3LYP with Grimme dispersion correction and with the basis set 6-31G(d,p) of calculations, on the homolithic rupture of covalent bonds 1-5 in the naphropane in the gas phase and in the carbon-containing nanocomposite (see Fig.). For the model of the outer surface of the CNT, the graphene-shaped $C_{48}H_{18}$ gross plane is selected, which is proportional to the size of nylon dimer.

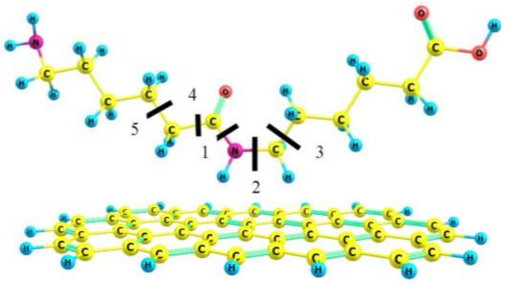

Fig. Nanocomposite model of kapron - CNT (shown covalent bonds whose energy was investigated)

The energy of the break of the covalent bond was calculated according to the formula: $\Delta E=(E_{tot}(A)+E_{tot}(B))-E_{tot}(AB)$, where $E_{tot}(A)$ and $E_{tot}(B)$ are total energies of fragments of nylon dimer, $E_{tot}(AB)$ is the total energy of nylon dimer. When considering ΔE values in a nano-composite, it was taken into account that the distance between one and the other fragments of nylon from the outer surface of the CNT is alternating.

The analysis of the results of quantum chemical studies shows that, regardless of the chosen covalent bond in the nylon dimer, the presence of a carbon nanotube fragment increases the energy of these covalent bonds (the value of the binding energy is given in kJ/mol):

Bond N in nylon	ΔE (gas phase)	ΔE (CNT-fragment 1)	ΔE (CNT-fragment 2)
1	447.1	509.8	486.0
2	430.5	475.4	487.5
3	363.7	406.6	433.8
4	384.5	414.1	463.0
5	376.8	397.4	467.9

In the formed nanocomposite nylon-CNT fragment the energies of all the investigated covalent bonds significantly increase as compared to that of pure nylon, which indicates an increase in the thermal stability of this nanocomposite. The indicated calculations are confirmed by the experimental data [1].

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Microemulsion synthesis of CeO$_2$ nanoparticles and their properties

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Oxidative stress, which often appears as a result of chemotherapy or irradiations, can lead to many serious diseases such as radiation sickness, Alzheimer disease *etc*. Therefore, search of biocompatible nanomaterials, which will be able to overcome the oxidative stress, i.e., demonstrate antioxidant activity is the important issue for scientists nowadays. From this point of view, cerium dioxide nanoparticles (CeO$_2$ NPs) are of particular interest because they can demonstrate antioxidant activity by the mechanism of several enzymes presented in human body [1].

This study devoted to synthesis of CeO$_2$ NPs by precipitation in the reversal microemulsions based on three surfactants (Triton X-100, CTAB and Brij-35).

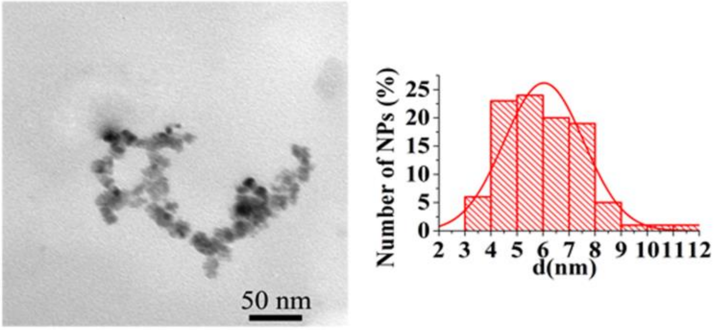

Fig. Representative TEM-image and particles size distribution for CeO$_2$ NPs synthesized in the reversal microemulsions based on CTAB

According to X-ray diffraction data, it has been established that CeO$_2$ NPs have the crystalline structure, which forms during the synthesis. As the results of TEM microscopy, it has been calculated that the average sizes of NPs are approx. 6.2 ± 1.5 nm and NPs have the narrow size distribution (Fig.). It was found that CeO$_2$ NPs have the high values of ζ-potential in the aqueous solution (+37 - +47 mV) that points on their high stability in the aqueous suspensions. Obtained NPs are promising for performing further biological investigation.

1. C. Xu, X. Qu, NPG Asia Mater. **6** (2014) e90-16.

Diffusion and rotation of clean >Ge=Ge< and mixed >Ge=Si< addimers on bucled face Si(001)(4×2)

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Epitaxial deposition of germanium on the relaxed face Si(001)(4×2) is intensively investigated both by experimental methods and by methods of modern quantum chemistry. This is due to the exceptional value of the corresponding process for the microelectronic industry. Special attention is paid to the earliest stages of growth of the surface layer, at which metastable structures are formed. Their configuration, stability, and dynamics of transformations contain important information not only on the adsorption and diffusion of adatoms, but also on the processes of nucleation, growth, and transformation of metastable nonepitaxial structures into epitaxial islands.

In the work method density functional theory (B3LYP, 6-31G**) has been employed the diffusion and rotation of pure >Ge=Ge< addimer formed during epitaxial deposition of germanium on the face Si(001)(4×2) and mixed addimer >Ge=Si<, the formation of which occurs during the mutual exchange of a Ge atom with a Si atom of the substrate. The relaxed face Si(001)(4×2) was modeled by the $Si_{28}H_{28}$ cluster, representing a series of five bukled surface dimers >Si=Si< with a 12° angle of backing. It has been established that the rotation of addimers >Ge=Ge< and >Ge=Si< from the non-epitaxial configuration A to the epitaxial B occurs as a result of the correlated motion of the atoms of the addimers with a significant elongation of 3.3 Å to one of their bonds with the substrate, but with the coupling remaining in the addimer. For the activation energy of rotation, the values of 0.74 and 0.86 eV are obtained respectively. Consideration of the rotation of addimers as rigid rotators leads to higher values of activation barriers.

The diffusion of both types of addimers from one cell of the cluster to the next is accompanied by a significant lengthening of the dimeric bond and the separation in time of the individual motion of the adatoms formed in this process. Transition states have configurations in which one of the addimer atoms is in one of the cells of the cluster, and the second is in the next. Evaluation of the activation barriers for diffusion displacement gave the values 0.85 (>Ge=Ge<) and 0.92 (>Ge=Si<).

Synthesis of nanosized organic-inorganic perovskite films $CH_3NH_3PbI_3$: effect of initial reagents ratio on formation and microstructure

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The development of cost-effective and highly efficient renewable energy sources is one of the greatest challenges for the 21st century. One of the promising renewable energy sources is the solar energy. Organic-inorganic perovskites have attracted considerable attention because it is inexpensive materials with high efficiency of energy conversion, their manufacturing is relatively simple and universal [1]. The complex chemical interaction of organic cation, the coordinating solvent and inorganic component affects the formation of crystals and the properties of materials, and requires a detailed study.

The aim of this work was to study the microstructure and phase transformations at the synthesis of organic-inorganic perovskites films $CH_3NH_3PbI_3$ at different ratios of the initial reagents.

Initial reagents PbI_2 and CH_3NH_3I with different ratios (1:1, 1:2, 1:3) were used for synthesis of organic-inorganic perovskites films. It was established that at the synthesis of films with ratio of PbI_2:CH_3NH_3I=1:1, the microstructure of the film is represented by anisotropic needle-like particles, with PbI_2:CH_3NH_3I = 1:2 – particles in the form of maple leaf, and with PbI_2:CH_3NH_3I=1:3 – the particles become more isotropic, the film becomes denser.

Organic-inorganic perovskites films $CH_3NH_3PbI_3$ with different ratios of initial reagents are formed according to different schemes: without the formation of intermediate compound (1:1), by formation of one and two intermediate compounds – $CH_3NH_3)_2PbI_4$ (1:2) and $(CH_3NH_3)_3PbI_5$, $(CH_3NH_3)_2PbI_4$ (1:3). In the ratio of initial reagents (1:1) organic-inorganic perovskite is formed at 70-80 °C, at a ratio of 1:2 and 1:3 at 170 °C and 175 °C, respectively.

The obtained results allow us to conclude that microstructure of organic-inorganic perovskite film is determined by microstructure of parent compound PbI_2 in case of initial reagents ratio 1:1, and the microstructure of the intermediate compounds $(CH_3NH_3)_2PbI_4$ and $(CH_3NH_3)_3PbI_5$ at the ratio of 1:2, 1:3, respectively.

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Natural components based environmentally friendly ionic polyurethanes

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Polymers based on renewable raw materials attracted a great attention of scientists due to three main reasons: the environmental issue, realization that oil resources are exhaustible and biocompatibility We have developed methods for synthesis of (bio)degradable oil/(exo)polysaccharide containing ionic polyurethanes with a high content of natural ingredients: castor oil (CO) and xanthan (Xa), which reduces the use of oil resources by 60% and improves the ecological state of the environment. The introduction of a significant amount of natural ingredients into the base ionic polyurethane (IPU) gives it the ability to degrade under environmental conditions at the end of its lifetime. Both hydrogen and covalent bonding between system's components ensures the destructive processes for the complete system as a whole, opposite to base IPU. The weight loss of IPU/CO/Xa during the incubation into the soil for 6 months in 1.86 times exceeds the actual content of natural ingredients. Study of material degradation in model environments showed that weight loss in an alkaline medium (at CO content of 50%) exceeds that of base IPU in 240 times. At simultaneous content of CO and Xa, the films at all were braking into the pieces.

X-ray studies have established the absence of the manifestation of Xa amorphous-crystalline structure in IPU/CO30/Xa20 that has proved the intermolecular interactions between components. The presence of natural components in basic IPU increases the strength properties of material in three times. It was shown that the structural, operational properties and degradability of studied polymers are determined by the structure and content of the natural components.

Film forming IPU/CO/Xa dispersions are perspective as biologically active substances in agriculture: immunostimulants and protective coating for seeds and plants; antitranspirantes for reducing water scarcity and optimization of the production process of crops in drought conditions; binders for biologically-active substances granulation. The advantages of such material lies in environmentally friendly production technology due to the absence of organic solvent, economy through the use of cheap renewable raw materials, reducing the harmful impact on the environment through the regulated level of (bio)degradation after the expiration of lifetime.

Zeolite anion-containing nanoporous materials, prospects their production and use

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The expansion of the use of natural zeolites raised the question of its modification and adaptation to current problems. Anionic forms of zeolites are of particular interest, since modified with anions (NO_3^+, PO_4^3, HPO_4^2) zeolites can be successfully used in agriculture. In addition, the use of enriched with anions (SO_4^2, HSO_4, CO_3^2) zeolites as an additive to building materials has a great future.

Zeolites belong to the group of cation-exchangers and their enrichment with cations is not difficult, and in the case of anions the process is complicated. We have proposed a new nanotechnological method for producing anionic substitutes. This method is based on the introduction of the desired anion-containing salt into the nanoporous structure of the zeolite (by melting) so that the material does not lose the zeolite structure and acquires the properties of an anion-exchanger due to the formation of a new phase. After the introduction of such materials into the desired system, due to the molecular sieve properties of zeolites, there is a gradual transition of anions into this system. All this contributes to the effective long-term use of the material obtained.

Bactericidal adsorbents obtained by ion exchange modification of natural phillipsite

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Earlier [1] bactericidal adsorbents with a high content of silver (230 mg/g) and zinc (86 mg/g), and later copper-containing phillipsite (66 mg/g) were obtained by ion exchange between natural phillipsite and salts of bioactive metals in the solid phase. Silver-containing phillipsite is characterized by the most powerful antibacterial activity, but copper and zinc-containing forms are quite active despite the fact that the amount of Cu^{2+} and Zn^{2+} ions released into the aqueous solution does not provide the minimal inhibitory concentration toward target bacteria *E. coli*. Apparently, the modified phillipsite samples, like some other zeolites [2], themselves exhibit the bactericidal activity, while the natural phillipsite is absolutely inactive.

Ion exchange reactions do not change the crystal structure of the zeolite, this is confirmed by the powder X-ray diffraction patterns and FTIR spectra preserving characteristic peaks, as well as by water sorption measurements at room temperature. The low-temperature N_2 adsorption-desorption isotherms demonstrate the presence of slit-shaped pores in non-rigid aggregates of particles and possibly well-defined cylindrical pore channels in natural phillipsite, almost unchanged in its modified forms, some changes in the crystallite morphology were fixed by scanning electron microscopy (Fig.)

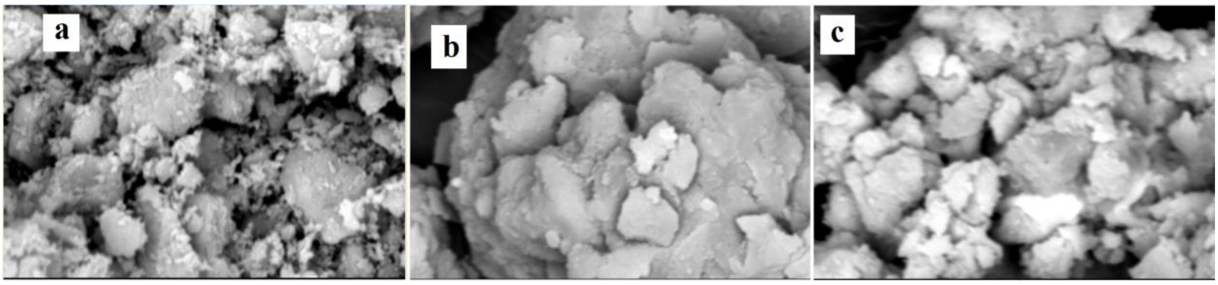

Fig. SEM images with magnification 5500 of natural phillipsite from Shukhuti (*a*), zinc-containing form (*b*) and silver-containing form (*c*)

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Role of sorption in flocculation process

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Chitosan and sodium alginate have physico-chemical properties: biodegradability, reaction and complexing ability, compatibility with living tissues without toxicity. Researches had shown that chitosan and sodium alginate can be used for flocculation of suspensions, sorption from aqueous solutions of heavy metals, surfactants.

Sorption has a specific role in the flocculation process with using chitosan and sodium alginate. Sorption is determined by the nature, molecular weight, concentration, charge density of the flocculants, as well as the properties of dispersions. It is necessary to understand the mechanism of processes in these systems in order to select an effective flocculants.

Researches are devoted to studying adsorption activity of natural polymers chitosan and alginic acid salts in aqueous solutions. Chitosan that obtained from shells of crustacean used as a flocculant. The equations of Langmuir, Hill – De Boer, BET were used for the description of adsorption. Our researches have shown that surfactants quite good adsorbed by natural polymers. The adsorption isotherms of anionic surfactants concerned to *L*-type, isotherms of cationic surfactants adsorption - to *S*-type.

The mechanism of action of natural flocculants is different from synthetic ones. The state of biopolymers depends on the pH of the solution. A positive effect on flocculation exerted by the addition of inorganic substances, surfactants or oppositely charged polyelectrolytes. The aim of our researches was to study the role of sorption in flocculation processes.

It was studied sedimentation stability of suspensions ground sediments containing macromolecular substances (flocculants) and surfactants. It was shown that the sedimentation stability defines as flocculants characteristics such as molecular weight, concentration, nature of flocculants, polyelectrolyte’s charge density and nature of the suspensions. It was found that compositions of natural flocculants chitosan and sodium alginate with surfactants are effective. The findings suggest that the studied compositions of natural flocculants have significant potential for use, due to a number of advantages: the efficiency of their actions, low reagent consumption, environmental safety.

An efficient synthesis of nitriles and nitrile-containing pharmaceuticals

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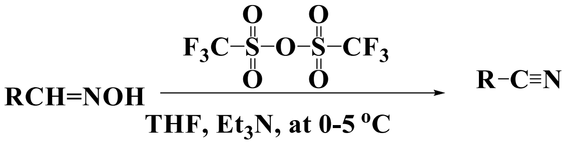
Over 30 nitrile-containing pharmaceuticals are prescribed for a diverse variety of medicinal indications with more than 20 additional nitrile-containing leads in clinical development. The prevelance of nitrile-containing pharmaceuticals and the continued stream of potential agents in the clinic attest to the biocompatibility of nitrile functionality [1].

In this study, a new and convenient protocol for the transformation of aldoximes to a nitrile is one of the most important reaction in organic synthesis. This transformation, which proceeds using trifluoromethanesulfonic anhydride (triflic anhydride: TA) and triethylamine, allows the conversion of a range of aldoximes, including aromatic aldoximes, heterocyclic aldoximes, acrylo aldoximes, aliphatic aldoximes, and cycloalkyl aldoximes, and the yields of nitrile are good to excellent [2, 3].



R = aryl, heteroaryl, cycloalkyl, alkyl, allyl

Fig. Synthesis of different substituted nitriles from aldoximes using trifluoromethanesulfonic anhydride

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The Diels–Alder reaction as an effective approach for the functionalization of the surface of carbon materials

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Carbon materials (CM) are among the most common materials due to their mechanical, chemical and adsorption properties. CM have been widely used for various applications such as catalysis materials, electrochemistry, sensors, biomedical applications, and so on. In particular, surface modification of CM by supporting specific functional groups can dramatically change the adsorbate-activated carbon interactions. Therefore, it is important to predict and control the final chemical structure of the carbon surface that usually can not be achieved by classical modification techniques. On the other hand, the Diels-Alder reaction is a selective method for CM functionalization.

The purpose of our work is the surface modification of activated carbon (SCN) by barothermal method with maleic anhydride (MA). The important criteria for choosing this dienophile is the presence of oxygen heteroatoms in MA molecule. Created functional groups (Fig.) can be used as adsorption and catalytic centers. The SCN-MA was characterized by N_2 adsorption, TG/DTG, TPDMS, FTIR and Boehm titration methods.

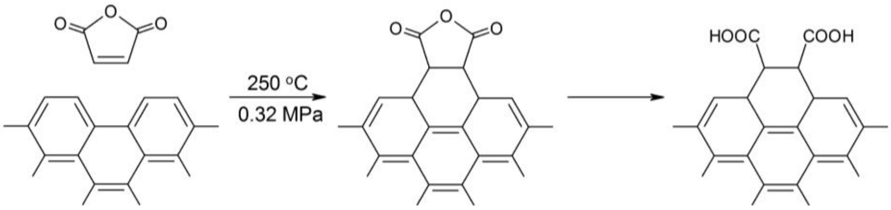

Fig. The scheme of the surface modification of SCN with maleic anhydride

It is shown, that SCN-MA in comparison with initial SCN is characterized by the significant mass loss effect in the temperature range 150-600 °C. This effect corresponds to the destruction of MA forms that were chemisorbed on the SCN surface. The slight reduction of this thermal effect after vacuum and alkaline treatment is explained by the removal of physically adsorbed and hydrolytically non-stable centers of MA. The process of pyrolysis in the surface layer of carbon materials modified with the Diels-Alder reaction was studied by TPDMS. It is proved that as a result of modification the chemisorbed forms of MA are formed.

So, as a result of barothermal modification of SCN by maleic anhydride is grafting of 2.0-2.2 mmol/g thermally stable carboxylic groups with a maximum desorption at $T > 350$ °C.

Adsorption of Co^{2+} cations and radioactive ^{60}Co by mesoporous TiO_2

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^{60}Co is one of the few anthropogenic, gamma-emitting radionuclides, that can be detected in aquatic environments affected by liquid effluent discharged from nuclear facilities. Although cobalt is an essential trace element, it is toxic when concentration levels are too high. Zeolites, resins, Fe_3O_4, nanosilica or aluminum silicate are proposed for adsorption removal of Co^{2+}. The need for control of the content of ^{60}Co in the environment, determines the search for new adsorption materials with high adsorption capacity.

In present investigations, we use a new mesoporous TiO_2 with a chemically modified surface for the adsorption of Co^{2+} and ^{60}Co from aqueous solutions.

The dependences of adsorption value from agitation time, solutions acidity, equilibrium concentration of Co^{2+} were investigated in batch mode. Four simplified kinetic models: Lagergren's pseudo-first and pseudo-second kinetic models, diffusion and Elovich kinetic models were applied to experimental data. The diffusion model provided better correlation than other kinetic models, except pseudo-second kinetic model. Equilibrium is established after 40-50 minutes of interaction between TiO_2 and solution of Co^{2+} due to high sorbent's surface. Experimental measurements of adsorption capacity of mesoporous TiO_2 towards Co^{2+} cations reached 2.5 $mmol \cdot g^{-1}$. These values are much higher than that for other adsorbents, describe in literature sources. Langmuir and Dubinin-Radushkevich adsorption theory applied for experimental equilibrium data. The adsorption energy was measured using Dubinin-Radushkevich equation. It was equal 9.26 kJ/mol, which corresponds to the mechanism of physical adsorption. To simulate conditions close to real, the radioactive isotopes of ^{60}Co were obtained using reaction: ^{59}Co (n,γ) ^{60}Co. Pu (α) Be compound was used as a source of neutrons ($\varphi=1.3\cdot10^6$ $n/cm^2\cdot s$; $E_n=1\text{-}10$ MeV). The sample activity detected by scintillate spectrometer with NaI(Tl). Decontamination factor, measured as the ratio of the activity of the solution of ^{60}Co before and after adsorption, is equal 0.98 (Fig.). Investigated mesoporous TiO_2 could be useful in decontaminating of radioactive waste containing ^{60}Co.

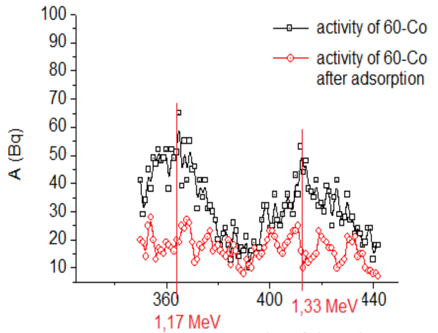

Fig. Part of gamma spectrum of ^{60}Co (interval of energy of gamma-quanta 1-1.5 MeV)

Antimicrobial properties of hydrogels/silver nanoparticles composites for surgical use

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Bacterial contamination is one of the problems of treating wounds of different etiologies. In response to the intensive use of antibiotics, bacteria have developed protective mechanisms that reduce the effectiveness of these drugs. Prospective candidates with bacteriostatic and bactericidal features are nanoparticles of metals and their oxides. Silver nanoparticles are ones of the most widely used. Their action mechanism is disrupting function of bacterial plasma membrane. Therefore, they are effective against Gram-negative and Gram-positive bacterial cells and can replace broad-spectrum antibiotics. The hydrogels with a porous structure which filled with silver nanoparticles are promising materials for the treatment of open wounds.

In present investigation the Polyacrylamide cross-linked hydrogels with different concentrations of silver nanoparticles were used. Initial Ag+ concentrations (M) in hydrogels of 10^{-4}, $0.5\cdot10^{-3}$, 10^{-3}, $0.5\cdot10^{-2}$, 10^{-2} were used for AsNPs preparation. Diffusion method on the Mueller-Hinton agar with cultures *Staphylococcus aureus* and *Escherichia coli* which have Gram-positive and Gram-negative structures of cell wall respectively was used for investigation of antibacterial activity. Disks with ceftriaxone were used as a control variant. Bacterial cultures were incubated at 37 °C for 24 hours.

Obtained hydrogels loaded with silver nanoparticles show the inhibition of the bacteria growth of both species.

The efficiency of hydrogels for trophic ulcers venous genesis was studied. No side effects were noted: pain, maceration of the skin, itching. The initial tests results were considered as good.

Consequently, the results indicate the possibility of cross-linked polyacrylamide hydrogel as an effective agent for prevention the bacterial contamination and treatment of wound and ulcers.

Catalytic decomposition of organic/inorganic peroxides by carbon matrix: experimental and quantum-chemical investigation

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The use of carbon materials as catalysts in hydrogen peroxide decomposition (HPD) reaction in aqueous media has been the subject of much consideration. However, relatively little attention has been paid to reactions of organic peroxides (in particular, benzoyl (BPD) and lauroyl (LPD)) degradation in organic solvents. The present work aims to clarify of the relationship between the surface chemistry and catalytic activity of carbon matrices in peroxides decomposition and to establish the plausible mechanism of these reactions.

For experimental study, activated KAU-type carbon (AC) and its oxidized (O-AC) form have been used. As nitrogen-containing AC (N-AC) SCN-type samples were explored. The catalytic activity of the carbocatalysts was detected by measuring the volume of released gases in the HP, BP and LP decompositions for 30 min at room temperature. The calculation was performed using the DFT method with B3LYP exchange-correlation functional and 6-31G(d,p) basis set.

Obtained results demonstrate that rate constants for HPD are in 3-4 orders more than for BPD and LPD (Table). According to experimental data, the activity of the carbon matrix is raising in the raw: N-AC >> AC ≥ O-AC, that is in good agreement with quantum-chemical calculations. However, according to the calculated data the most exothermic reaction is BPD (probably because of π-π conjugation of BP molecule with carbon matrix), that does not correspond to experimental kinetics. Obviously, besides energy effects, other parameters (such as surface area, porosity, diffusion) also influence the catalytic process.

Table. Experimental and calculated data of the HPD, BPD and LPD decomposition

Experimental data: rate constant $k \cdot 10^{-6}$ (s^{-1})			
	HPD	BPD	LPD
AC	2850	0.66	0.60
O-AC	2230	0.15	0.80
N-AC	4330	1.10	5.70
Calculated data: reaction energy (ΔE, kJ/mol)			
AC	-43.514	-55.032	-13.420
O-AC	-43.515	-57.331	-13.930
N-AC	-119.630	-77.650	-26.970

Technology for the production of complex products based on celsian ceramics

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Ceramic radiotransparent materials, which combine dielectric properties with high mechanical characteristics and high thermal resistance (more than 1000 °C) at a low density (up to 3200 kg/m^3) are perspective materials in the creation of aircraft technology. The creation of radiotransparent materials with a complex of high performance characteristics and the development of technological parameters for the manufacture of parts of various shapes and sizes is an urgent need of the modern aerospace industry.

In previous studies, we obtained the optimal composition of ceramics based on the crystalline phase of the Celsian ($BaAl_2Si_2O_8$). The formulations of celsian ceramics within the elemental triangle «SiO_2 –$BaAl_2Si_2O_8$–$BaSi_2O_5$» of the $BaO – Al_2O_3 – SiO_2$ system are localized. Physical-chemical and electrophysical properties of synthesized materials are determined in laboratory conditions. The possibility of obtaining monophasic celsian ceramics at a reduced synthesis temperature (1350 °C) with a low dielectric constant ($\varepsilon < 7.6$) and the tangent of the angle of dielectric losses $tg\delta\ 10^{-3} = 5.5$ has been established.

The obtained data testify to the suitability of the use of the developed ceramics as radiotransparent materials used in the manufacture of parts for aircraft. Subsequent studies are aimed at establishing technological parameters for obtaining products of complex shape while maintaining specified strength characteristics.

Synthesis, photo- and electrocatalytic properties of nanostructured TiO_2-Ce films

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Titanium dioxide is a promising material for application in environmental photocatalysis, for the generation of electricity in the solar and fuel cells, gas sensors, optical and protective coatings, electrochemical devices, as oxygen reduction catalyst *etc*. The catalytic activity of titanium dioxide increases greatly when nanoparticles are used. We present the results of the study of photo- and electrocatalytic properties of electrodes based on nanostructured titanium oxide films modified by Ce.

Electrocatalytic films based on nanodispersed titanium oxide modified by Ce were produced by sol-gel method on Ti substrate from solutions containing titanium isopropoxide, ethanol, acetic acid, cerium nitrate and surfactant (Triton X-100); after which the electrodes were annealed in air at 500°C. The prepared samples were characterized by using X-ray diffraction and ultraviolet-visible photocurrent spectra. The average size of nanoparticles was no more than 11 nm. The XRD results indicated that TiO_2 and TiO_2/Ce electrodes calcined at 500°C consisted of anatase as the unique phase. The photocurrent spectra of the TiO_2/Ce electrodes ($0 \leq$ Ce concentration ≤ 2 mol%) showed a stronger current in the UV range and a shift in the flat-band potential (E_{fb}) towards more negative values than that of TiO_2 electrodes.

Electrocatalytic properties of TiO_2 and TiO_2/Ce electrodes were investigated in the processes of oxygen electroreduction. It has been found by *I-E* curves measurements that the potential of oxygen reduction changes with the film composition. It is shown that modifying of TiO_2 films by cerium improves catalytic activity of TiO_2/Ce electrodes (Ce concentration up to 2 mol%) in the reaction of oxygen electroreduction, that appears in decreasing of oxygen reduction potential E_{O2} and increasing of dynamic range of O_2 electroreduction potentials ("electrochemical window"). The high electrocatalytic activity of TiO_2 nanoparticles in the oxygen reduction process may be due to the formation of catalytically active Ti^{3+} centers and to the presence of OH groups in the oxide matrix.

The electrodes investigated were distinguished by a high sensitivity to dissolved oxygen [$(4\text{-}5)\cdot10^{-6}$ g/l] and high reproducibility of characteristics in long-time cycling. These electrodes promise much as reusable electrode materials in electrochemical sensors for the determination of oxygen in liquids.

Operando studies of the catalytic and gas sensing properties of nanostructured copper and tin oxide layers

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The nanostructured layers exhibit large surface-to-volume ratio with high concentration of active surface sites for chemisorption. In this study, we report on the synthesis of copper oxide and tin oxide nanostructured layers and their application as a gas sensor. SnO_2 nanostructured layers were prepared by pulsed laser deposition while CuO_x nanowires were obtained by the thermal oxidation method. Scanning electron microscopy (SEM) and atomic force microscope (AFM) were used to characterize the morphology of the as-prepared oxides. A simple gas sensors were realized by depositing of SnO_2 and CuO_x on a special fused silica substrates and were investigated *in operando* under exposure to the reactive atmosphere at elevated temperatures by means of Near Ambient Pressure XPS (NAP-XPS) [1, 2]. We were able to follow the resistivity of the nanostructured films simultaneously with NAP-XPS measurements during the gases exposure. The unique combination of thin film resistivity measurement and photoelectron study under higher pressure of investigated gases brings a new insight into a sensoric properties and catalytic processes on the surface.

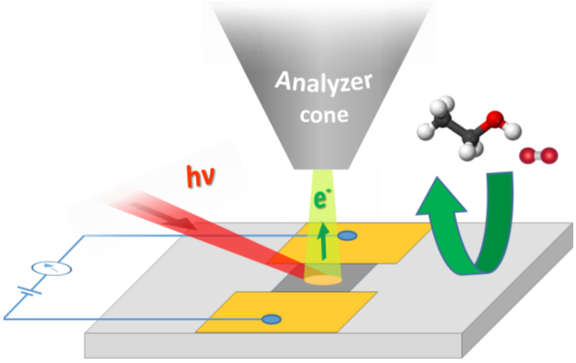

Fig. Combined NAP-XPS and resistance measurements

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Impact of modified polymers (polyacrylamide and starch) on kaolinite electrokinetic potential

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Zeta potential allowed to explain the inter-particle interactions occurring in the colloidal system as well as solid tendency to aggregation. Polymers added to the suspension may affect this parameter. Usually macromolecular compounds form long structures on the solid surface (‘loops’ and ‘tails’) that influence the slipping plane position and charge [1].

In this paper the effect of various modified polymers on kaolinite zeta potential value was examined. For the experiments, anionic and cationic forms of polyacrylamide and starch were selected. Zeta potential was measured using a zetasizer Nano ZS (Malvern Instruments). In Fig. the results obtained in the presence of anionic (AN) and cationic (FO) polyacrylamides are presented.

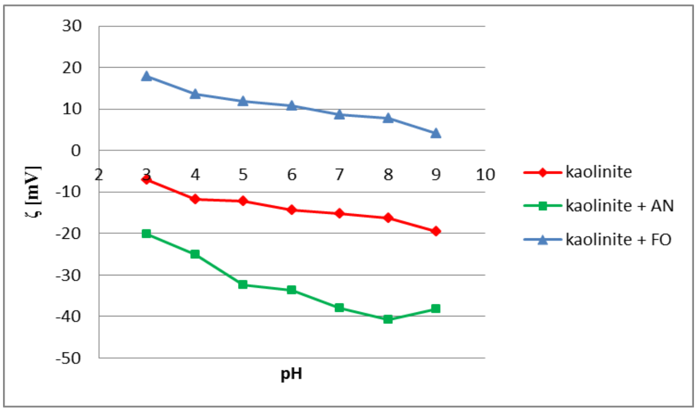

Fig. Electrokinetic potential of kaolinite particles in the absence and presence of anionic (AN) and cationic (FO) polyacrylamide

Kaolinite particles without macromolecular compounds have negative potential value in the whole examined pH range. Cationic polymer makes the ζ values more positive, in turn anionic polymer – more negative.

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Mixed oxides with different composition as adsorbents of polymeric substances from aqueous solutions

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Polymers soluble in the aqueous medium find a wide usage in many branches of industry, medicine, environmental protection and agriculture. They are applied as dispersants, foaming agents, thickeners, flocculants and modifiers of the solid surface properties. The following polymers belongs to this group of macromolecular compounds: poly(acrylic acid) – PAA, poly(vinyl alcohol) – PVA and polyacrylamide – PAM. These polymers can be successfully used as agents changing surface characteristics of both simple and mixed oxides. Taking into account the morphological and microstructural properties of mixed oxides (also these nanosized), mechanical strength and non-toxicity, as well as wide possibilities of their modifications, these materials have a lot of interest in recent years. In many cases the application possibilities of metal oxides are limited due to inadequate surface characteristics. The appropriate surface modification (i.e. by adsorption of high-molecular compounds) leads to obtaining solids with the properties desired in specific processes.

The main aim of presented studies was comparison of adsorption affinity of selected mixed oxides (SA: SiO_2-Al_2O_3, ST: SiO_2-TiO_2 and AST: Al_2O_3-SiO_2-TiO_2) for synthetic polymers (PAA, PVA and PAM) soluble in aqueous medium [1-3]. The effects of metal oxide content in the oxide material and solution pH were examined. Based on the adsorption and electrokinetic (solid surface charge density, zeta potential) results, the more probable mechanism of polymeric macromolecules binding with the mixed oxide surface was proposed. It was shown that specific composition of mixed oxides influences significantly the amount of adsorbed polymer and the structure of polymeric layer formed at the solid/liquid interface.

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Dielectric properties of hybrid carbon-based composite materials and composites with titanium dioxide

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Composite materials consist of a polymeric matrix and conductive fillers. They are widely used in industry applications: electronics, electromagnetic shielding, conductive coatings fabrication for aerospace construction, in semiconductor devices *etc.* [1]. A considerable task is to obtain a low percolation threshold to reach and preserve optimal mechanical properties of polymers using a minimal concentration of fillers. To achieve this goal so-called synergy effect works, which is known, in particular, for multiphase composites. Thus, the study of dielectric parameters provide important knowledge about the polarization mechanisms, which occur in materials under applied AC field and, in general, about the charge transport process in composites [2].

In this work we compare the dielectric/electric properties of composites filled with different types of conductive carbon fillers and with dielectric titanium dioxide. To determine the dielectric properties of composites at low frequencies (namely, 100 kHz), we used a capacitor method based on measuring the capacitance of investigated samples. Measurements were performed using multifunction digital device APPA-703.

The dielectric/electric properties of epoxy composites filled with carbon nanotubes (CNTs), graphite nanoplatelets (GNPs), titanium dioxide (TiO_2) and mixed titanium dioxide / graphite nanoplatelets, carbon nanotubes / graphite nanoplatelets are compared across a wide concentration of fillers range from below the percolation threshold to well above it. The highest value of dielectric permittivity is observed in composites with carbon nanotubes only. However, the dielectric properties of composites filled with GNPs are also very attractive. It was demonstrated that the dielectric and electric properties of composites with GNP filler can be substantially improved with the addition of CNT and TiO_2 due to the synergy effect. In composites with inclusions of mixed titanium dioxide / graphite nanoplatelets, carbon nanotubes / graphite nanoplatelets, the dielectric permittivity increase due to the decreasing of the average distance between nanocarbon clusters.

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Adsorbable organic halogens as wastewater contaminants

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Adsorbable organic halogens (AOX) is the sum of organic halogen compounds (chlorinated, brominated and iodinated organics) in different environments – water, soils, sludge, sediments and industrial discharges that can be adsorbed on activated carbon. Most of them are toxic, mutagenic and carcinogenic at high concentrations, have long half-life period and high lipophilicity and can accumulate in food chains. AOX can be found in different environments, but mainly in industrial wastewaters, e.g. wastes from pulp and paper industry, pharmaceutical, dyeing and chemical industries, landfill leachates, agrochemicals (insecticides and herbicides), steel industry and biofuel production *etc*. Thus, there are limits for AOX presence in pulp and paper industry wastes: China – 0.72 kg/tp, Canada – 0.25 kg/tp, the USA – 0.272 kg/tp, in territory of European Union - 0.25 kg/tp [1]. In European Union there are several standards for AOX determination - ISO 9562:2004 and U.S. EPA Method 1650 with further microcoulometric detection of inorganic chloride. The samples need to be pretreated. It includes: acidic pH of solution ($pH<2$), maintained by nitric acid, elimination of oxidizing agents influence by adding of sodium sulfide and samples storage by 8 h in these conditions to loose of chloride from microorganisms and algae. For sorption of AOX different activated carbons can be used as a sorbent.

The commercially available granular activated carbon (GAC, ITES Vranov, s.r.o.) was examined for AOX sorption from model aqueous solutions that contain 4-chlorophenol, 4-bromophenol and 4-iodophenol as standard compounds. Content of halogenphenols before and after adsorption was recorded by UV-Vis spectroscopy. The main conditions for adsorption were determined: pH 6.2, agitation time 240 min, adsorbent dosage 50 mg/25mL. pH was maintained by mixing of 0.1 M sodium citrate and 0.1 M nitric acid. Under optimized conditions GAC removal efficiency is Q_{max}= 164.71 mg/g for 4-chlorophenol at concentration level 411.3 mg/L. Future investigations are aimed to determine the adsorption capacity of 4-bromophenol and 4-iodophenol on GAC.

Acknowledgements
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Formation of nanoporous bioactive coatings by anode oxidation method

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Titanium and titanium alloys are widely used for implants production, but they have no complete bone integration and reactive bioactivity properties. Different surface modification techniques have been used to improve bone tissue integration due to the formation of intermediate porous layer suitable for osteoblasts [1]. In this work the uniform porous TiO_2 films on Ti (BT 1-0) were obtained by anodic oxidation. Initially the samples were mechanically polished to a mirror finish and cleaned by ethanol solution. For anodic oxidation process, 0.5 M H_2SO_4 solution was used as electrolyte. It took place in two-electrode electrochemical cell using Ti plate (area is 0.5×2 cm^2) as anode and Pb as cathode electrode. The process was carried out using DC power supply applying 229 V. Various time (10 or 30 minutes) and amperage (from 4 to 70 mA) were used. Morphology of porous TiO_2 oxide film (I=70 mA) is shown in Fig.

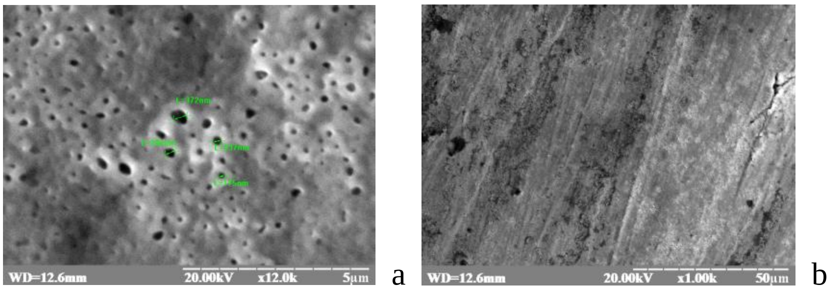

Fig. Morphology of TiO_2 coatings obtained in 0.5 M H_2SO_4 solution,
I=70 mA, U=229 V, 30 min (*a* –x12.0 k and *b* –x1.0 k)

The obtained pores have a mean diameter from 175 to 372 nm. Close results were obtained for Zr/Nb implants in the same electrolyte. The best porous coatings were obtained after 10 minutes at 70 mA.

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Hydration of alginic acid and the influence of the hydrophobic environment in the presence of hydrochloric acid

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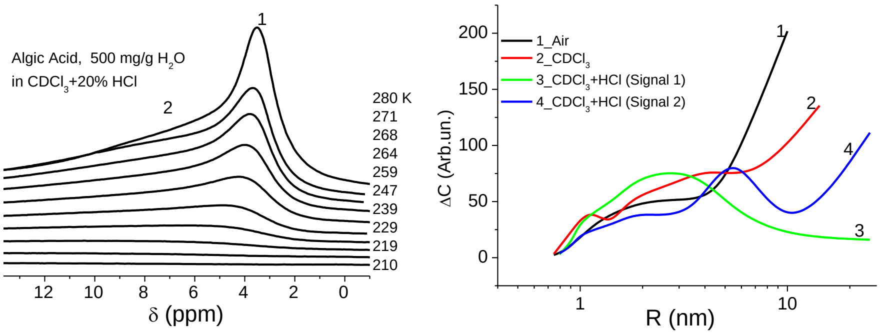
Alginic acid (AA) is widely used in the food industry as an effective thickener capable of binding large amounts of water. In addition, AA has bioactive properties and is used in many medicinal and cosmetic preparations.

The purpose of the work was to determine the thermodynamic and structural characteristics of water adsorbed by solid polymer AA with a total content of 500 mg/g in the sample, as well as the effect on the bound water of the medium of a weakly polar organic solvent - $CDCl_3$ and hydrochloric acid addition. The measurements were carried out by the method of low-temperature ^1H NMR spectroscopy.



a b

Fig. The ^1H NMR spectra of water adsorbed by alginic acid (C_{H2O} = 500 mg/g) taken at different temperatures in $CDCl_3$ with HCl added (*a*) and distributions along the radii of clusters of adsorbed water for hydrated AA in different environments (*b*)

It is established that all water in the air is strongly associated and is observed in the spectra in the range of chemical shifts of 5–8 ppm (Fig., *a*). The environment of chloroform reduces the average associativity of water and the chemical shift decreases to 4 ppm. The addition of HCl leads to the appearance in the spectra of two signals differing in the value of δ_H. The signal in a strong field (3.5-5 ppm) refers to water clusters that do not dissolve HCl.

Thus, the effective binding of water by the polymer prevents the adsorption of weakly polar molecules and leads to the formation of a significant number of water clusters that do not dissolve strong acid (HCl). The radius of such clusters is about 2 nm (Fig., *b*). They are probably formed in the gaps between the polymer chains of the polysaccharide.

Sorption properties on radionuclides ^{137}Cs and ^{90}Sr of compositions based on natural zeolite

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In conditions of high anthropogenic pressure on the environment, a number of harmful substances, including radionuclides, enter the human body. Accumulating in the body of radionuclides impede the normal development and functioning of the body, and in high doses cause irreversible changes. One of the ways of solving this situation is enterosorption. Oral use of enterosorbent drugs over a period of time allows both to prevent the flow of these substances into the human body, and to ensure their gradual removal from the body. The search and development of safe and effective means for the prevention and treatment of the negative effects of radionuclides on the human body is an important task of medicine and pharmacy.

The purpose of the work was to study sorption properties of compositions based on natural zeolite in relation to radionuclides ^{137}Cs and ^{90}Sr.

The sorption capacity of the samples relative to the radionuclides was studied using the static sorption method at 37 °C and at pH values 2.0, 5.5 and 8.0. Radionuclide solutions ^{90}Sr and ^{137}Cs were used without carriers. The radioactivity of the dry residue was measured using a radiometer α-β- automaton NRR-610 "Tesla". The statistical error of experiments did not exceed 5 %.

Adsorption of radionuclides on sorbents depends on many factors. Among them, the most important is the contact time of the solution with the sorbent. The highest rate of adsorption samples showed in the first 30 minutes and achieves adsorption equilibrium in heterophase system within 30-60 minutes from the start of the experiment.

Sorption properties of samples relative to radionuclides are more dependent on the acidity of the solution. It is better the slightly hydrated ion of cesium is absorbed, the strontium ion, which has high values of the thermodynamic characteristics of hydration, is much less absorbed. This dependence of the sorption value on the pH of the solution confirms the literature data that the zeolites are weakly acidic polyfunctional ion exchanges, and sorption is carried out according to the mechanism of ion exchange.

Modification of nanoporous structure and surface of carbon materials to be used in energy storage technology

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The project is aimed at enhancing the performance of electrochemical double layer capacitors (EDLC), which successfully penetrate more and more market niches like hybrid automobiles, light trains, wind turbines, consumer electronics, UPS-systems, defence industry, *etc*.

A few methods to modify the porous structure and surface of activated carbon materials have been developed, namely:

- an increase in pore width due to thermal treatment in a tube furnace of the microporous carbon material containing formic or oxalic acid absorbed;
- an increase in pore width due to microwave treatment (800 W - 9 min) of the microporous carbon material containing oxalic acid absorbed;
- modification of a nanoporous carbon surface with nitrogen heteroatoms as a result of thermal treatment of a dry mixture of carbon and melamine powders either in a tube furnace or in a microwave oven.

It has been found that both conventional thermal treatment and microwave treatment give similar results, though the latter requires much less time and energy consumption. The effectiveness of N-atom modification of the carbon surface in nanopores was verified by its catalytic activity in the H_2O_2 decomposition – see Figure wherein curves 1 and 2 show the activity of ZL carbon before modification, while curves 3 and 4 illustrate an increase in activity after modification with 5 or 10% of melamine (M). Besides, the performance of EDLC prototypes is also improved if the modified carbon is used in electrodes.

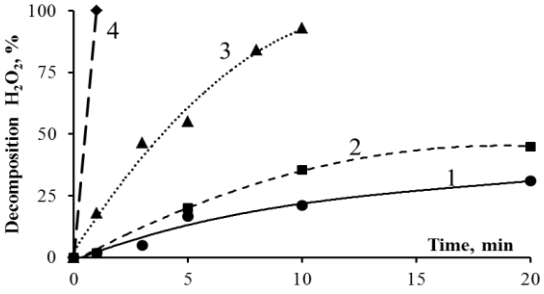

Fig. Catalysis of H_2O_2 decomposition. *1*- ZL as is; *2* – ZL-800W-9min; *3* - ZL+M 5%-800W-9min; *4* - ZL+M 10%-800W-9min

Both types of modification, namely, an increase in pore width and N-doping the surface, result in reducing the internal resistance of EDLC prototypes and in some cases also in increasing their working voltage from 2.7 to 3.0 V. These two factors can provide the corresponding increase in power capability and energy density, in particular, under high loads.

In cooperation with Yunasko-Ukraine Company, the EDLC prototypes of various capacitance and voltage were manufactured, the prototypes demonstrating the best performance as compared with those known on the market.

Synthesis and characteristics of iron-containing nanocomposites based on palygorskite

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The aim of this work is synthesis of iron-containing nanocomposites based on organopalygorskite for extracting ions of heavy metals from aqueous environment. As the object of the study we took natural silicate – palygorskite of the Cherkassky deposit, which has formula ($Mg_5Si_8O_{20}(OH)_2(H_2O)_4 \cdot 4H_2O$) [1].

The following chemically pure reagents produced by the company (Merck): $FeSO_4 \cdot 7H_2O$, hexadecyltrimethylammonium bromide (HDTMA) and sodium borohydride ($NaBH_4$) were used in the experiments. Palygorskite (PG) was cleaned from impurities by the method of sedimentation of coarse dispersed phase. Organopalygorskite (OPG) was obtained by modifying the surface of PG by the cation surface active substance HDTMA [2].

The synthesis of nano-dimension zero-valent iron (nZVI) was carried out without the use of inert atmosphere by the techniques described earlier [3] with some modifications. Reduction of iron is performed by reaction:

$$Fe^{2+} + 2BH_4^- + 6H_2O \rightarrow Fe^0 + 2B(OH)_3 + 7H_2\uparrow.$$

The excess of BH_4^- in the reaction amounted to 30 % of stoichiometric amount according to the equation of reaction. The resulting nano-dimension iron was separated from the liquid phase by centrifugation, washed three times with alcohol and dried under vacuum at temperature of 80 °C. Similarly the iron-containing nanomaterials, where OPG and PG were used as substrates, were synthesized.

It was found that the synthesized composite extracts up to 45 mg/g of ions of Co(II) and 18-45 mg/g of ions of Cr(VI), which is much more efficient in comparison with the iron-containing sorbents that do not contain surface active substances.

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The biological effect of stabilized silver nanoparticles on pathogenic hospital microorganisms, the healing process of open wounds and the growth of winter wheat

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Traditional biocide preparations for medicinal, industrial or everyday applications are based mainly on organic substances, which are toxic for humans and environment and cause different allergic reactions, side effects and resistance. Therefore, the biocide preparations of a new generation comprised metal nanoparticles with a wide antibacterial, antiviral, and antifungal action, are of special interest. It is very important that the microorganisms' cells are usually not capable of producing resistance to these "nanobiocides" or "nanoantibiotics". Recently, metal nanoparticles have been actively used also in the practice of growing agricultural plants.

In the present work, we studied the effect of new biocide compositions based on silver nanoparticles (AgNPs) and silica/polyacrylamide hybrids on a number of bacterial and fungal cultures, which are traditional hospital infections, as well as the compositions' ability to heal wounds and to affect the growth of winter wheat. In the first experimental series, we used as free biocide compositions as fragments of cotton fabric impregnated with these preparations. The investigated AgNP compositions demonstrated a high bactericide action against the bacteria *Staphylococcus aureus, Escherichia coli,* and *Pseudomonas aeruginosa,* fungicide effect on black yeast-like fungus *Exophiala alcalophila* and fungistatic effect on yeasts *Candida albicans* and filamentous fungi *Aspergillus ustus, Cladosporium shpaerospermum* and *Fusarium oxysporum*. The fungistatic action of the compositions on *F. oxysporum* lasted up to 30 days.

The compositions demonstrated also a high activity in the full skin cut wound healing in rats. In addition, they fully prevented the inflammation of the wounds, which is characteristic in the first 3 days. Thus, these biocide preparations can widely be used for the treatment and prolonged disinfection of wound dressings, sanitary materials, and clothes.

It was shown a significant effect of the compositions on the life cycle of winter wheat plants in the case of pre-sowing treatment of their seeds.

Investigation the diffusion regime in a porous medium by spatiotemporal scaling of the diffusion coefficient

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The diffusion in porous media may be Fickian or anomalous. The anomalous diffusion is usually characterized by the two parameters, particularly, by the anomalous diffusion coefficient and the anomalous diffusion exponent, contrary to the standard diffusion approach, which admits only the standard diffusion coefficient. Depending on the diffusion regime the mass transfer rate may be either faster or slower compared to the standard Fickian diffusion. Herein, we present an approach for estimation of the diffusion regime by the diffusion coefficient scaling.

The methanol and the methane transport in the mesoporous zeolite-alumina pellet was studied. Varying the pellet's size and the diffusant amount, the values of the diffusion coefficients were estimated. Previously, it had been demonstrated that the methane transport through the zeolite-containing pellet is described by the Fickian diffusion equation, whereas the methanol transport is described by the non-Fickian diffusion equation with either space-time-fractional or time-fractional derivative. In this respect, for calculating the diffusion coefficients, the standard diffusion and the time-fractional diffusion models were used for the methane and the methanol respectively. The relations between the obtained values of the methanol non-Fickian diffusion coefficients ($0.0068 – 0.0276\ \mathrm{cm}^2/\mathrm{s}^\alpha$) measured for unequal pellet sizes and various diffusant amounts were found to follow the temporal scaling with a fractional exponent equal to 1.17±0.03, which corresponds to the time-fractional diffusion equation, in a concise manner. It supported a conclusion that the anomalous diffusion of the methanol is time-fractional. An essential applicability of the approach based on the analysis of the temporal diffusion coefficient scaling was additionally verified using the standard Fickian diffusion coefficients of the methane ($0.00094 – 0.00376\ \mathrm{cm}^2/\mathrm{s}$). Critical analysis of the spatial scaling for both, methanol and methane, demonstrated that it is inapplicable in the experimental scenario studied. Investigating the spatial scaling requires the knowledge of the real diffusion length which cannot be estimated using the experimental technique utilized in the current investigation.

Synthesis and characterization tetra-acid complexes of anesthetic preparations

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Local anesthetic drugs with pharmacological and therapeutic potential were selected as ligands in the process of searching for new biologically active complexes. According to the chemical structure, local anesthetics are divided into two groups: esters and amides. In particular, novocain is ester, and lidocaine and trimekain refer to amide. The presence of a nitrogen atom of amide and amine groups and an oxygen atom of carbonyl groups are determined the donor properties of ligands and their ability to produce complex compounds.

Chlorides of metals and hydrochlorides of anesthetic preparations, recrystallized from aqueous solutions were used for the synthesis of complex compounds. Whenever necessary, insoluble forms of preparations (Lid, Tm, Nov) were obtained by a known technique. The experiment was carried out in water, water-ethanol solutions and various organic solvents or in their mixtures. The optimal parameters (solvent, pH of solution, temperature) were established for the original method of syntheses.

Preparation of complexes had been investigated in various metal-ligand stoichiometric ratios. It was established that at any initial metal-ligand ratio composition of complex compounds is respectively 1:2. Therefore, the following complexes were obtained: $(AnsH)_2\,[MeCI_4]\cdot nH_2O$, where Ans = Lid, Tm, Nov; Me = Cr(III), Ni(II), Fe(III), Sn(II), Cd(II) (in the case of lidocaine hydrochloride), Ni(II), Zn(II), Mn(II), Cu(II), Fe(II) (in the case of trimecain hydrochloride), Cr(III), Ni(II), Zn(II), Mn(II), Cu(II), Fe(II), Fe(III), Sn(II), Cd(II), Co(II) (in the case of novocaine), $n = 0, 1, 2$.

The composition and individuality of the synthesized coordination compounds was established by elemental analysis, melting points; physical-chemical properties of compounds was studied by X-ray diffractometric, thermographic, IR spectral methods; Also, solubility of synthesized complex compounds in water and organic solvents as well as their electrical conductivity in water environment have been studied.

Acknowledgements

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Kinetic and equilibrium of sterol adsorption on composite materials

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The new nanocomposites are an example of the preparation of new functional materials. Among them, nanocomposites based on commercially available materials, as well as natural polymers such as chitosan provides obtaining materials with advanced physicochemical properties and new possible applications. The properties and behaviour of organic molecules on the surface of a solid body are of fundamental importance in modern applications and developed technologies. Integration of elements from the field such as biological sensors, organic electronics, and integration of bio and nanotechnology. Although the knowledge of small molecules on the surface is exhaustive, there are still problems understanding the adsorption of larger molecules of biological importance due to their complexity.

In this work, the chitosan/silica (CS/silica) composites as well as silica and carbon materials were prepared and used as potential adsorbents of sterols (cholesterol). Cholesterol concentration in experimental samples was determined by chromatographic methods (HPLC) and spectrophotometric method. Experimental measurements were performed for the purpose of adsorption efficiency, including the size of the adsorption capacity and the kinetics of this process. On the basis of the obtained results, the relations between the properties of the adsorption system and the efficiency of adsorption processes occurring were determined. The obtained results compare the level of adsorption state for selected systems. In order to more fully describe the cholesterol adsorption process on selected adsorbents, the kinetics of the adsorption process was analysed. These results suggest the preferred cholesterol adsorption on the chitosan composite (Fig.).

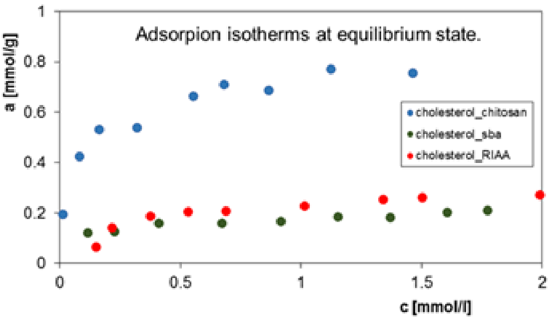

Fig. Cholesterol adsorption isotherms performed at equilibrium state

SAXS investigation of the composite materials

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Nanocomposites are one of the type of nanotechnology products with a constantly growing importance, mainly due to the possibility of modifying and adapting properties to specific applications. Biocomposites create a new generation of multi-element materials. A lot of effort is given to the development of sustainable and environmentally friendly methods of obtaining and processing nanocomposites. Small angle X-ray scattering (SAXS) can be applied to analyse the structural changes in composite matrix after any modification. Scattering patterns can be obtained due to the crystal structures (particles) are present in samples. In general, the nanocomposite systems and also the system investigated in this work include the crystalline, amorphous and background regions with characteristic electron densities. When the differences in electron densities are significant, the significant changes in the SAXS spectra are observed. In this work, SAXS investigation of various composite samples were presented. The investigated samples varied in the intensity of scattering. The intensity of the scattering signal was the largest for the biopolymer nanofibers (chitosan) modified by silver ions and the smallest for material without silver nanophase. It is the first evidence that some changes in the nanocomposite structure that have occurred when silver nanophase was incorporated (Fig.). This reveals a single correlation between the size of the silver nanophase and X-ray scattering at small angles and may suggest the properties of nanoparticles in/on the nanocomposite body. To quantify these changes, the values of the sizes of electron density inhomogeneity were calculated.

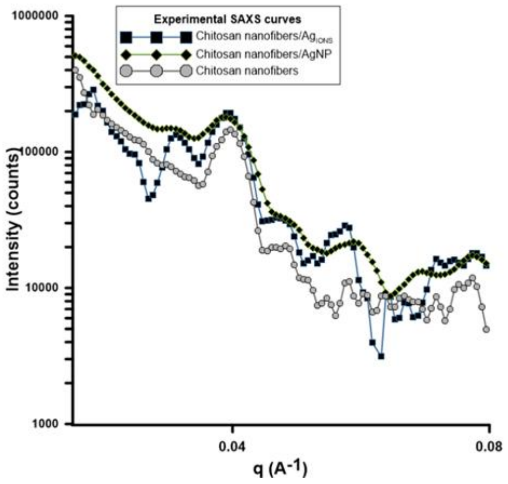

Fig. Experimental SAXS profiles for chitosan nanofibers, chitosan nanofibers modified by silver nanoparticles and chitosan nanofibers modified by silver ions

Spectral properties of ultra-dispersed systems of LaF_3 and EuF_3 in the stiffened melt NaCl-KCl

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Saline melts are very convenient media for the synthesis of various materials, in particular, nanostructured systems. This paper presents the results of studying by spectral methods: IR transmittance spectroscopy, diffuse reflectance (DR) spectroscopy, luminescent spectroscopy of solidified solutions-melts of LaF_3 and EuF_3 in the saline system NaCl-KCl. A preliminary assessment of fluoride solubility on the basis of thermodynamic calculations of exchange reactions in the melt gave values of about 0.74 and 0.29% by weight, respectively, for LaF_3 and EuF_3 at 700°C. The first of the values is consistent with the data of quantitative X-ray diffraction analysis (~1%). IR spectra of solidified solutions-melts contain a clear band in the range of 250-260 cm^{-1}, corresponding to NaCl, and a less expressive band at 206-210 cm^{-1} (KCl). At the same time, the IR spectra of the undissolved residues also contain bands in the range of 360-390 cm^{-1}, corresponding to the Ln–F bonds. The DR spectra of LnF_3 in NaCl-KCl contain a deep band in the negative region at 245 nm, which corresponds to the intrinsic luminescence of NaCl, in the absence of its own absorption bands of La^{3+} ions. An analogous band is observed in the EuF_3 DR spectra in NaCl-KCl, while it overlaps with the luminescence excitation band of Eu^{2+} at 350 nm. These bands are also contained in the DR spectra of the undissolved residue, while their intensity is much lower. In the range of 1800-2200 nm, in this case, the absorption band characteristic of Eu^{3+}, consisting of several peaks of different intensities, also manifests itself. The possibility of a redox reaction between Eu^{3+} and Cl^- ions is shown. The solubility of EuF_3 according to XRD data is about 2%. The luminescence spectrum of LaF_3 in saline melt is a broad band of middle intensity with a maximum at 460 nm. In the case of salt melt with EuF_3, the luminescence band has the form of a rather narrow peak of high intensity with a maximum at 430-440 nm. In addition, a low-intensity emission band is detected, consisting of several peaks in the range of 500–700 nm, which is due to its appearance to electronic $4f$ - $4f$ transition in Eu^{3+}. A similar absorption band takes place in the undissolved residue, while its intensity is much higher.

Analysis of the properties of some photorefractive organic materials for dynamic holography

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Recently, photorefractive (PR) organic materials began to gain popularity, especially their properties for dynamic holography. The analysis was carried out of the properties of some materials that are particularly attractive stand out from the rest of the materials: PC61BM:Alq3:PTAA:PDCST:TAA (tris(8-hydroxyquinolinato)aluminium) composite and C60:PbS:PATPD:PVK:7-DCST:ECZ (doped PbS nanocrystals in molecular triphenyldiamine photosensitized with C_{60}, composite). For C60:PbS:PATPD:PVK:7-DCST: ECZ, we have a response speed of 399 μ, for PC61BM:Alq3:PTAA: PDCST:TAA - 860 μ [1]. It is known that the shorter the response time, the clearer the dynamic update of the recorded 3D image will be. Studies have shown that these materials have the following features: C_{60} as the photosensitizer, PbS gives avoiding the detrimental effect over PR efficiency; low dielectric constant, high optical nonlinearity and easy processing, Alq3 gives trapping sites for electrons and thus forms a competing gratings via separate transport.

For dynamic holography, in turn, we need the following characteristics: $\tau \approx 10^{-9} - 10^{-10}$ s (this is due to the fact that the speed of processing information in a computer is large); efficiency of dynamic holographic material should be around 80 - 90 %; also exist other important parameters (sensitivity, *etc*.), but problems with them successfully can be resolved. The bottom line is that the parameters of these materials are included in this framework, if not completely, then indirectly. As analyzed, most of the materials that were previously used for dynamic holography do not have such indicators, which lead to the conclusion that it is nanocrystals that are embedded in structures that are crucial. Nanoparticles such as PbS, C_{60}, Alq3, QCdS, QCdTe, and others can be potentially important for the development of this type of material. It is also worth noting that the best indicators have molecules that are composed with S and Cd. It is important to note that all materials are PTAA(poly(triarylamine)) or PVK(Poly(9-vinylcarbazole))-based PR composites. By assumption, success in building a material that will have all the necessary properties and is also convenient in industrial production will consist of the following elements: plasticizer - ECZ = N-ethylcarbazole, as a polymer - PTAA or PVK, as a sensitizer – molecules with S or molecules C_{60}.

1. J.-S. Moon, K. Kim, D.-W. Han, *et al*., Appl. Spectrosc. Rev. **222** (2017) 203.

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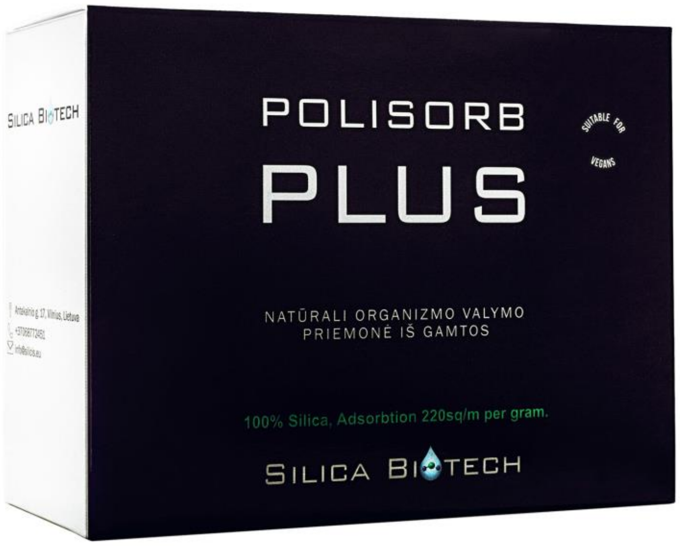

Dietary supplement “Polysorb Plus” is designed to cleanse human body. The product adsorbs various harmful substances that are built up in the intestine with the following their excretion from the body.

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