Machine Learning-Driven Analysis of Carbon Nanotube Accumulation in Cancer Cells via Raman Spectroscopy

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Machine learning offers significant potential for extracting insights from extensive datasets. In this study, we utilized principal component analysis (PCA) and K-means clustering to explore the accumulation of single-walled carbon nanotubes (SWCNTs) in cancer cells. We examined the Raman spectra of cells exposed to SWCNTs capped with either DNA or oligonucleotides (ON) and tracked their temporal evolution. Through unsupervised machine learning techniques, we elucidated the mechanisms and sequences of SWCNT accumulation and distribution in glioma cells, highlighting the chirality discrimination by capping molecules and subsequent selective intracellular transport. PCA facilitated the denoising of Raman spectra and extraction of specific biochemical information, while K-means clustering visualized the distribution of nanotubes and cellular compartments. Utilizing machine learning, we successfully extracted information on carbon nanotube accumulation in cancer cells from Raman spectra datasets, obviating the need for additional research methods.

Self-organization of charged particles in lateral potentials with a high symmetry

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The problem of the optimal configuration of a finite number of particles in a plane has been a difficult problem of both physics and mathematics for many centuries. Back in 1611, Kepler posed the question of why a snowflake has perfect hexagonal symmetry [1]. At present, increased interest in the problem of the optimal configuration is also due to the development of nanotechnologies which make it possible to form systems of similarly charged particles confined by external potentials with a high symmetry. For example, this problem arises when analyzing the behavior of quantum vortices in a Bose condensate [2]; electrons in quantum dots [3]; and the self-organization of colloidal particles at the interface between two different liquids [4, 5].

In this communication we discuss the basic principles of self-organization of one-component charged particles, confined in disk and circular parabolic potentials [6,7]. The main idea is based on the cyclic symmetry and periodicity of the Coulomb interaction between particles located on several rings. Our approach reduces significantly the computational effort in minimizing the energy of equilibrium configurations and demonstrates a remarkable agreement with the values provided by molecular dynamics calculations. With the increase of particle number $n \geq 180$ we find a steady formation of a centered hexagonal lattice that smoothly transforms to valence circular rings in the ground state configurations for both potentials. At the same time, the energetic preferences for nonuniform local density then favor ground states where this locally hexagonal structure is isotropic dilated and contracted throughout the structure. In fact, the equilibrium configuration is determined by the need to achieve equilibrium through the formation of a hexagonal lattice on one side and a ring-like structure on the other. This competition leads to the formation of internal defects in such systems, in contrast to the case of unlimited regions, where the ground state of the system has no defects [8]. Finally, this structure smoothly transforms to valence circular rings in the ground state configurations for both potentials.

We briefly discuss the precursors of the phase transition of the type “hexagonal lattice – hexatic phase” with the increase of a particle number in the system at zero temperature.

[1] J. Kepler, The Six-Cornered Snowflake (Clarendon, Oxford, 1966).
[2] H. Saarikoski, S. M. Reimann, A. Harju, and M. Manninen, Rev. Mod. Phys. **82**, 2785 (2010).
[3] J. L. Birman, R. G. Nazmitdinov, and V. I. Yukalov, Phys. Rep. **526,** 1 (2013).
[4] B. P. Binks and T. S. Horozov, Colloidal Particles at Liquid Interfaces (Cambridge Univ. Press, Cambridge, 2006).