

Molecule modelers in 3D virtual laboratories

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Virtual laboratory is a software designed to model a chemical process, to change its settings and parameters, to demonstrate characteristic signs of chemical reactions, whether qualitative (textures, colors, precipitates, bubbles, flame, etc.) or quantitative (tables, plots, charts), or both. In contrast to distance laboratory – a telecommunication system used in chemical engineering to conduct real chemical experiments in a geographic location different from that of the experimenter – virtual laboratory is typical for chemical education. Being a vehicle for computer method of teaching chemistry, this software enables special means for implementing interactive instruction and often has an editor for developing new lab assignments.

Developed originally as self-contained software, virtual laboratories have been evolving into interactive Internet pages. They are growing increasingly popular as independent resources and as components of massive open online courses (MOOC). E. g. on www.ChemCollective.org one can set virtual experiments in laboratories of stoichiometry, thermochemistry, chemical equilibrium, solubility, oxidation-reduction, electrochemistry. A remarkable feature of the website is laboratory of forensics, in which students study chemistry investigating a staged crime scene. Along with other animations and simulations, websites of California State University collection of open and free net resources www.merlot.org and of American Chemical Society www.ACS.org provide extensive lists of virtual laboratories. Instructors and students, teachers and pupils do not have to download and install them – the laboratories are ready available for use online.

At all the diversity of themes, designs, and practical instructional values of virtual chemical laboratories, most of them remain two-dimensional (flat). This disadvantage is seldom experienced; however, in some topics of chemical science three-dimensional representation of objects is a paramount: configurations and conformations of organic compounds, molecular shapes of covalent compounds with various types of hybridization, spatial orientation of atomic and molecular orbitals. In a real-world classroom, the problem is solved using ball-and-stick or space-filling molecular models; sometimes an effective two-dimensional visualization can help, too. However, will it work in distance chemical education?

For all the above reasons, chemistry instructors are exploring educational affordances of three-dimensional (3D) virtual immersive environments like Second Life (SL). Students and instructors communicate in world in voice and text chat and act as avatars that can be modified up to photographic resemblance with the originals [1].

Over the last decade, the author has virtually replicated in SL buildings of University of Oregon Center for Advanced Technology in Education, UO Jordan Schnitzer Museum of Arts JSMA.UOregon.edu, Lane Community College www.LaneCC.edu. The author's recent work is replication of Madrone Hall in Linn-Benton Community College www.LinnBenton.edu with its physical and chemical laboratories, where one can run virtual chemical experiments.

Among the available functionalities (some of them were originally developed at Drexel University), one should mention molecule modelers (rezzers), didactically valuable for solving the aforementioned problems of three-dimensional representation when studying certain topic of chemistry. The college course of general chemistry includes valence shell electron pair repulsion theory (VSEPR). Students study molecular shapes as results of hybridization of atomic orbitals and repulsion of the molecular with lone electron pairs. The theory implies that this repulsion must be minimal. This 3D topic follows Lewis dot structures, usually drawn in 2D. It is logical to suppose, therefore, that a virtual 3D laboratory will be a more appropriate environment to consider objects in.

A simple molecule modeler in this virtual laboratory works as follows: rezzing a molecular template with a specific type of hybridization (trigonal planar for sp^2 , tetrahedral for sp^3 , trigonal bipyramidal for sp^3d , octahedral for sp^3d^2) → manipulating the central atom (specifying chemical element) → manipulating peripheral atoms (specifying chemical element) → manipulating the bonds (making them double or triple or a lone electron pair) → optional manipulating the molecule (ion, radical) as a whole (labeling and turning on rotation) → optional saving the molecule in the avatar's inventory for future use (demonstration, sharing with classmates, more close studying). A more sophisticated molecule modeler for complex chemical species works with thin files of compounds, prepared in HyperChem. When one puts the file content to the modeler, the molecule with bond lengths and angles optimized to minimum energy is rezzed instantly. Operating this modeler, students familiarize with basic cheminformatics.

A group of students can work with the same molecule modeler at the same time. Successful collaborative building in world requires coordination of activity and depends on psychological effects of immersion, presence, proteus, and communication by avatar's poses and gestures. Acquired in the virtual laboratory, these skills of working as a team will be of great importance for students' future real job in chemical research and industry.

References

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