Virtual Reality Chemistry: Computer Desktops Before Bunsen Burners

Eva Zurek
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CURRENT RESEARCH

Discovering new materials and chemical processes through theoretical and computational chemistry

What comes to mind when you think of a chemist? Probably beakers, volumetric flasks, bunsen burners, and pH meters. However, in the world of quantum chemistry, which is sometimes called computational chemistry or "virtual reality chemistry," chemists use computer simulations. Rather than watching chemical reactions in a sterile environment, computational chemistry is a desk job where chemical reactions and chemical species are analyzed, data is collected, and scientists are able to calculate and visualize molecular orbitals all from a computer desktop. This approach is advantageous because it ultimately results in general rules which can be employed by experimental groups to synthesize and design solids and molecules with desired properties for specific applications.

Dr. Eva Zurek, a quantum chemist at the University at Buffalo SUNY, conducts computer simulations, carried out with programs, which approximately solve the quantum mechanical Schroedinger equation. State-of-the-art computer facilities are used to: predict new materials for specific applications, uncover the relationship between structure, bonding and properties, reveal why a certain chemical species behaves the way it does, gain a more in-depth knowledge of a chemical system than is possible with experimentation, and help experimentalists interpret their results. Dr. Zurek's efforts decrease the time and effort required for experimentalists to develop new advanced materials and chemical processes. She is able to pave the foundation for experimentalists doing basic research to build upon her data to create wide ranging applications that will impact all of society.

Currently, Dr. Zurek and her team are using theory, modeling and...

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AFFILIATION

University at Buffalo, SUNY

EDUCATION

- Ph.D. in Chemistry 2006 ,University of Stuttgart
- M.Sc. in Chemistry 2002 ,University of Calgary
- B.Sc. in Chemistry 2000 ,University of Calgary
- B.Sc. in Physics 2000 ,University of Calgary

RESEARCH AREAS

Technology, Chemistry

FUNDING REQUEST

Your contributions will support Dr. Zurek's unique and collaborative work with chemists, physicists, and materials scientists to study new materials that will lead to the advancement of basic scientific research leading to innumerable applications, including new energy sources, alternative plastics, electronic applications, and geological discoveries. Donations fund the costs of salaries and stipends of Ph.D. students and postdoctoral fellows, computer hardware and software, and conference travel.

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