R & D facts

U.S. Department of Energy
Office of Fossil Energy
National Energy Technology Laboratory

Chemistry and Surface Science

08/2008

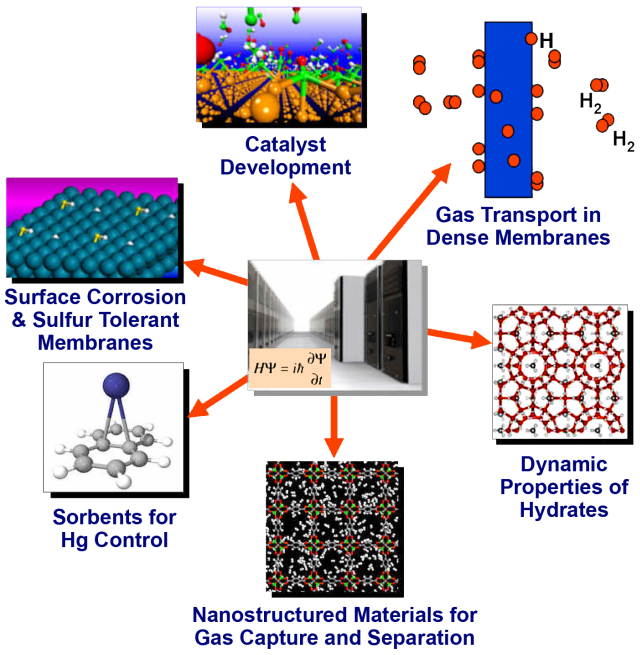
Computational Chemistry Research in Support of Future Energy Technologies

Background

Development of efficient future technologies for energy production with zero carbon emissions based on the use of fossil fuels or novel renewable resources is highly dependent on solving a large number of individual breakthrough tasks in diverse number of areas. These range from identification of new materials for gas capture, storage or separation to optimization of energy use and transformation processes. The overall goal of the NETL Computational Chemistry Group is to provide the atomistic insight into behavior of materials and chemical processes and correlate the atomic and molecular scale structure and property information to practical performances of materials and processing conditions of interest for various technologies developed at NETL.

Advancing Transformational Energy Technologies Through Scientific Discovery

The research done by Computational Chemistry Group at NETL is focused on investigation of a diverse number of systems and chemical processes ranging from catalysts development for fuels from coal (hydrogen and others), development of dense membrane systems with improved gas transport properties, surface corrosion, and fuel cell processes, to novel nanostructured materials for gas storage and separation (e.g. hydrogen separartion, CO_2 separation and absorption).



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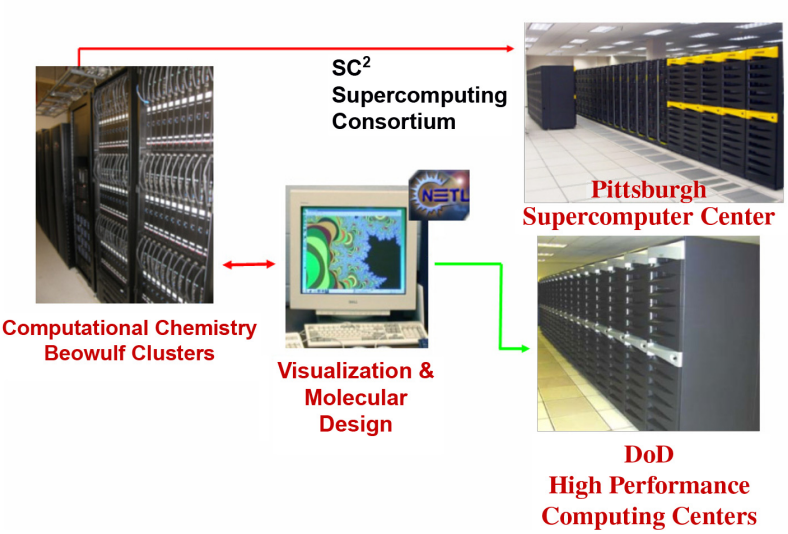
These problems are investigated using a variety of quantum and classical computational methods. Among the portfolio of computational chemistry capabilities used by the group are

- Ab Initio Molecular Orbital Calculations
- First Principles Density Functional Theory Calculations
- Classical and Quantum Molecular Dynamics Simulations
- Grand Canonical Monte Carlo Simulations
- Kinetic Monte Carlo Simulations

Based on these methods the group is able to provide unique atomistic information about the structural properties of bulk systems and their surfaces, stability and performance properties of bimetallic alloys, description of chemisorption properties in both homogeneous and heterogeneous processes or prediction of dynamical and transport properties in either gas, liquid or solid phases.

Computational Chemistry Facilities

NETL has developed state of the art computational and visualization facilities fully dedicated to the research activities performed by Computational Chemistry Group. These include a diverse number of Intel and AMD-based Beowulf cluster systems with modern communication capabilities like InfiniBand and Myrinet. Additionally, the members of the group perform research at Pittsburgh Supercomputing Center as members of SC2 (Supercomputing Science Consortium) and on a variety of supercomputing systems at various Major Shared Resource Centers within Department of Defense.



Academic and Other Government Research Collaborations

The fossil energy research conducted by Computational Chemistry Group at NETL is done in collaboration with the regional universities. Hands-on-training is provided to students and postdoctoral researchers interested in learning and applying computational chemistry methods to solve the large portfolio of problems in the fossil energy area. Additionally, the work done at NETL provides further support to the mission of Department of Defense in the development of new energetic materials and fuels.