

# How Do We Simulate Things at the Scale of Molecules and Electrons?

## An introduction to the Technology and HPC Aspects of Computational Chemistry

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### Abstract

*Computer simulations combined with high performance computing have benefited many areas of science and engineering. Chemistry is no different. Computational chemistry involves simulating systems at the atomic and electronic level. When examining individual molecules at this microscopic scale, quantum mechanical effects are important. As a result, to get the physics 'right' we need to solve the quantum mechanical Schrödinger equation or equivalent to properly describe these systems. In this presentation, a brief introduction to the technology of modern computational chemistry and molecular scale modeling will be given. Additionally, some examples how computational chemistry has provided important insights into chemical processes will be presented. A study of how anti-wear engine oil additives function at the molecular level in automobile engines will be provided (Mosey, Mueser, Woo Science, 2005, **207**, 1612) and our recent efforts to search in silico for new pure nitrogen analogues of diamond at high pressure will be given. (Phys. Rev. Lett. 2006, **97**, 155503)*