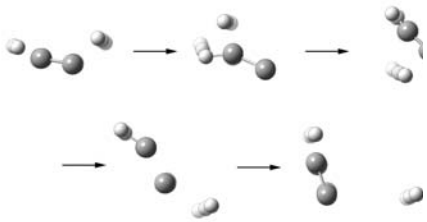
UNIVERSITY OF WASHINGTON

Computational Chemistry (Chem 465, Winter 2006)

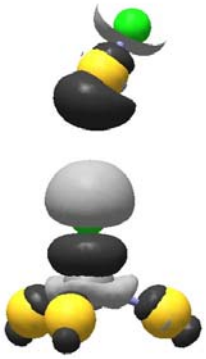
– A different type of experiment

Advances in computer engineering and software technology have extended the capability of computational chemistry from theoretical work on a few small molecules to a vast array of much larger systems including materials and biomolecules. Science and technology are greatly benefiting from the growth of computational chemistry in its multifaceted capability of modeling many aspects of chemistry.



Reaction dynamics of $C_2H_2^{2+}$

Chem 465 offered by the Chemistry Department focuses on applying electronic structure theories and molecular dynamics to the calculation of reaction properties including potential energy surfaces, energetics, electronic wave functions, and molecular conformations. Students will have a unique opportunity to develop interdisciplinary research subjects on their own. The goals of Chem 465 are



Electron density of $F_3CH\cdots FH$

- To provide some background on the theoretical and computational methods use in molecular modeling
- To provide hands-on experience with various molecular modeling software packages
- To provide an introduction to some current methods in molecular modeling
- To provide some understanding of the capabilities, limitations and reliability of various molecular modeling methods

The course will consist of two lectures and one computational lab per week. Course assignments will involve computations of chemical properties, reviews of papers from the scientific literature and a major computational project chosen by the student according to his/her research interest. Prerequisite: either CHEM 455 or CHEM 475, either of which may be taken concurrently; familiarity with Mac, Windows and Unix OS desirable but not required (we will go over the basics). Text books: *Introduction to Computational Chemistry* by F. Jensen (required), and *Essentials of Computational Chemistry – Theories and Models* by C. J. Cramer (optional).

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