Computational Chemistry

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1 Lecture 0 - Introduction to Course

1.1 What do we care about?

Things chemistry/materials-related:

- What are the properties of atoms?
- What molecules do they make? What other substances do they make?
- What are the shapes of those molecules? Structures of those solids? Properties of them?
- How do those substances react with each other?
- What are the energies of those reactions?
- What are the rates of those reactions?
- What is the strongest substance?
- How do we make a substance to do....?
- add your own questions....

Things that relate to the *chemical* properties of substances.

1.2 How are we going to figure these out? With only a computer?

1926: Erwin Schrødinger equation: $\hat{H}\Psi = E\Psi$

1929: Paul Dirac, British physicist

> The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus *completely known*, and the difficulty lies only in the fact that application of these laws leads to equations that are *too complex to be solved*.

It therefore becomes desirable that *approximate practical methods* of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.

1930's-1950's: Elaboration, analytical applications

1950's : Computers start to appear for technical applications

1960's-1970's: Numerical solutions of Schrødinger equation for atoms/molecules—expert users

1980's: "Supercomputer" era—routine use of computational chemistry software becomes possible

Figure 1: Ohio State Cray Y-MP supercomputer, ca. 1989. World's fastest computer at the time. 333 MFlop top speed, 512 Mb RAM.

1990's: "Chemical accuracy" era—very precise solutions routinely available, for a cost! See Schneider, *J. Phys. Chem.*, 1994.

1990's: Density functional theory (DFT) allows applications to solids/surfaces/liquids become common. See Hass, *Science*, 1998

1990's: Visualization moves to the desktop

2000's: Computational "screening", materials "discovery" See Greeley, *J. Phys. Chem. C*, 2009. Also see Gurkan, *J. Phys. Chem. Lett.*, 2010.

Today: Computational "chemistry" widely integrated into all aspects of chemical, materials, biological research

1.3   Our goals

"Computational chemistry" is now so vast it is impossible to cover everything completely. We limit ourselves to quantum-mechanics-based calculations.

1. Understand when it is appropriate to use quantum-mechanics methods.

2. Be able to state the basic theoretical, mathematical, and numerical concepts behind quantum mechanical wavefunction theory (WFT) and density functional theory, (DFT) calculations.

3. Understand the terminology and practical issues associated with doing quantum chemical simulations.

4. Get hands-on experience with these concepts using popular computational tools of today, including Gaussian for molecular systems and Vasp for condensed phase systems.

5. Learn how to apply the results of quantum chemical simulations to calculate things you care about.

6. Demonstrate an ability to formulate a problem and apply QM methods to it.

7. Develop the skills to understand a literature paper in the area.