

***Computational Nanoscience***  
***NSE C242 & Phys C203***  
***Spring, 2008***

**Lecture 15:**  
**In-Class Hartree-Fock Calculations**  
**March 11, 2008**

**Jeffrey C. Grossman**  
**Elif Ertekin**

# Quantum Chemistry Fun with Molecules...

- 1) Compute the total energy of the hydrogen atom.
  - How does it change with different basis sets?
- 2) Now compute the optimized structure and energy of the H<sub>2</sub> molecule.
  - How does the binding energy change with basis set?
  - How does the optimized H—H distance change with basis set?
- 3) Now let's do water.
  - What did you choose for the spin state of both H<sub>2</sub>O and the O atom?
  - What is the computed O—H distance and binding energy?
  - Do your results agree with experiment? Why or why not?
  - What is the gap of water and does it agree with experiment?
- 4) N<sub>2</sub> is one of the strongest bonds in nature\*.
  - How strong is it?
  - How does it compare with the CO bond?
- 5) Which are linear and which are straight/planar: CO<sub>2</sub>, NH<sub>3</sub>, BH<sub>3</sub>, NH<sub>4</sub><sup>+</sup>

\*speaking of which, this wouldn't be a bad time to review stuff like the chemical bond, e.g., at [http://en.wikipedia.org/wiki/Chemical\\_bond](http://en.wikipedia.org/wiki/Chemical_bond)