

# CHE 499 Independent Study: Research in Chemistry

## Theme: Applied Quantum Chemistry

Supervisor: Dr. Rod Macrae

This course is an alternative to CHE 360/460 (Co-op in Chemistry) and fulfils the research/professional practice component of the requirements of the BS. It is also a useful elective course for BA Chemistry majors, and for majors in Mathematics or Computer Science.

Quantum chemistry is the field of chemistry in which molecular structures and properties are calculated by direct numerical solution of the Schrödinger equation on a computer. The methods are known as *ab initio* methods because they require the use of no parameters other than the mass and charge of the electron, the masses and positions of the nuclei, and the overall charge and spin state of the molecule. The 1998 Nobel prize in chemistry was awarded to John Pople and Walter Kohn for developments in this field.

Several projects are available (see separate sheet).

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### Projects:

Vibrations, electronic spectrum, and donor-acceptor complexes of  $I_2$ .

Vibrations and hyperfine interactions of free radicals trapped in zeolites.

Hydrogen atom addition to ferrocene.

The trapping potential surface for hydrogen atoms in octasilsesquioxane cages.

Modeling the solid state based on exactly-solvable few-parameter potentials.

