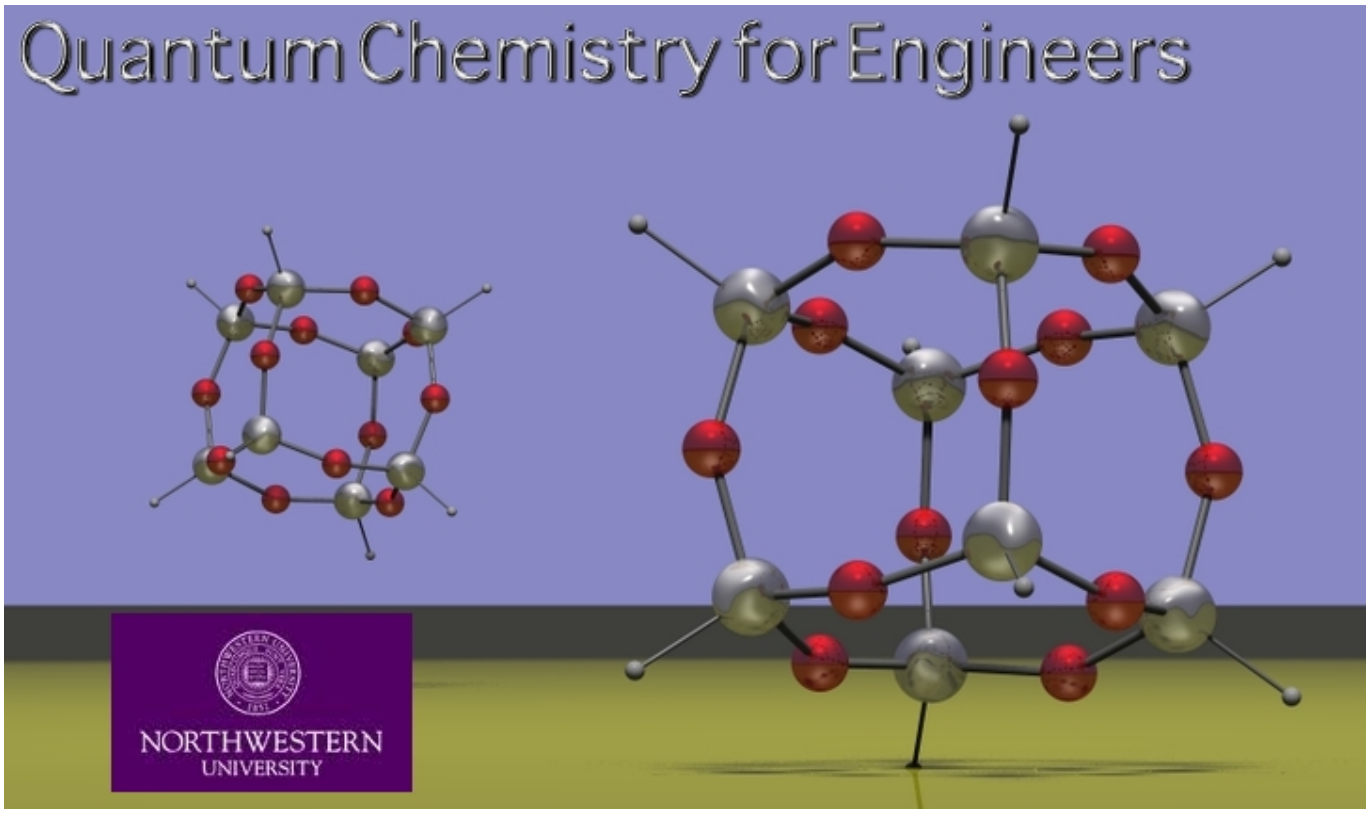
Quantum Chemistry for Engineers: Nanohub Nanoscience Projects



Electronic structure calculations play a major role in science and engineering, providing valuable information about molecular structure, thermodynamic and spectroscopic properties, and for modeling chemical reactivity and catalysis. The teaching of electronic structure theory at the undergraduate level is a common activity in chemistry departments (usually as part of a physical chemistry curriculum that is taught to junior-level students), and often some of the students are from engineering. Traditionally the material covered in such courses emphasizes fundamental concepts, such as the postulates of quantum mechanics, and simple applications, such as the particle in box, harmonic oscillator, and the hydrogen atom. Sometimes there is a computational component in which an electronic structure code is used to study small molecule properties. Such material is reasonable for chemistry majors, but does not serve engineering students very well.

At Northwestern University we have developed curricular materials for teaching junior-level engineering students that include projects with an engineering emphasis. These projects use the **NUITNS** program package at nanoHUB.org, which is an integrated package for electronic structure computation and molecular property visualization. **NUITNS** provides a user environment where the interface for defining the nature of the calculations and for visualizing the results is straightforward enough that the students can focus on the physical content of their calculations, basically making quantum mechanics “come alive” for solving problems that have

real-world connections.

NUITNS includes the following components:

* QC-Lab : electronic structure calculations based on the GAMESS electronic structure program (also includes the MacMolPlt and Molden programs for building and display of molecules)

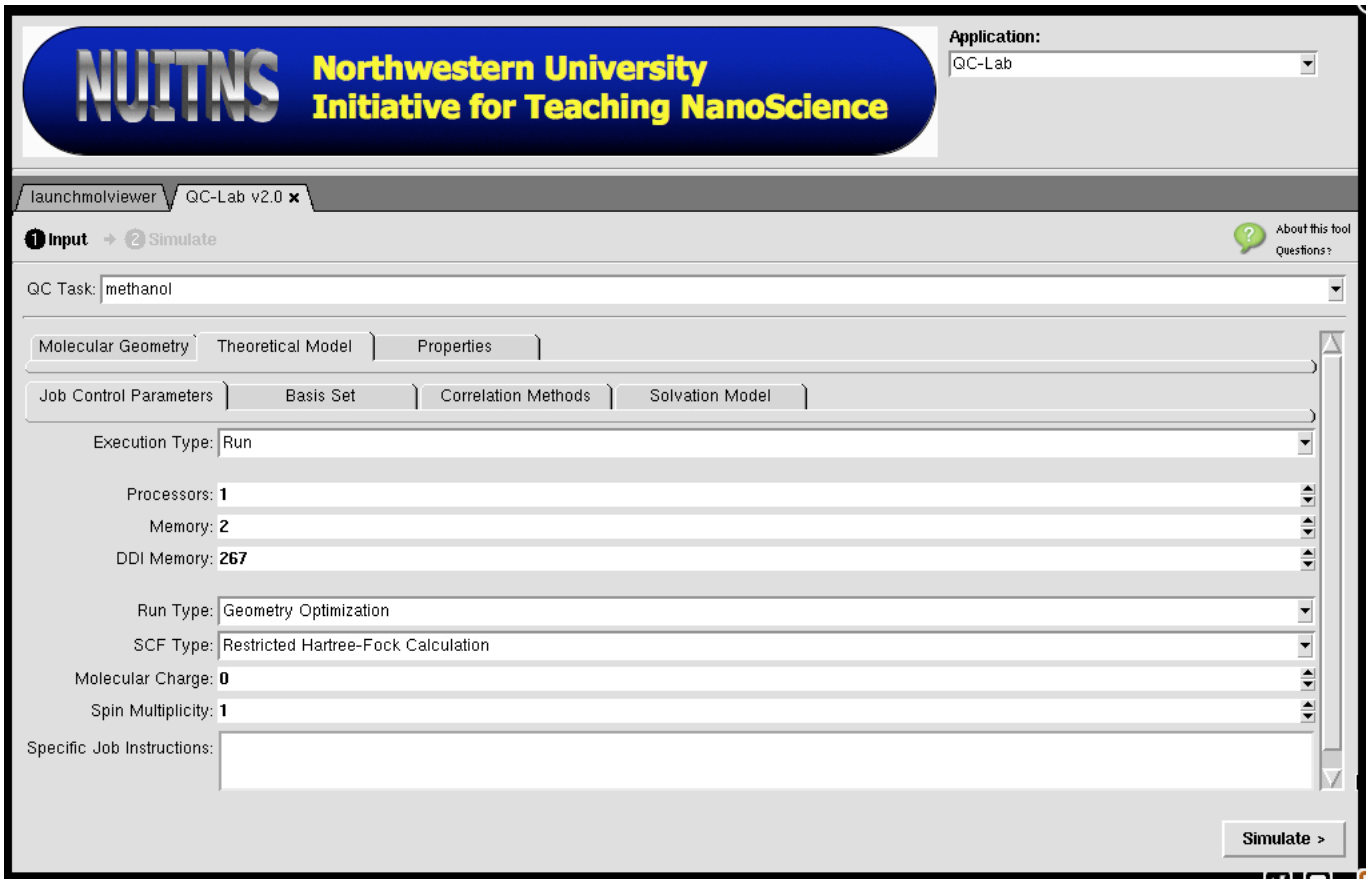
* CNDO/INDO : electronic structure calculations based on semiempirical methods

* UV-Spec : electronic structure and the prediction of electronic spectra based on semi-empirical methods

* MolST Molecular Structure Tracer: visualization of molecular structure

* TEDVis Theoretical Visualization of Electron Density: visualization of electron density

Among these components, **QC-Lab** provides the most extensive functionality for doing electronic structure calculations. The figure below shows a snapshot of the QC-Lab interface, which includes facilities for inputting or building molecular structures, defining parameters for using a variety of electronic structure methods and basis functions, and selecting many different properties to calculate. The output from such calculations can be used (via the MacMolPlt and Molden programs) to display molecular orbitals, electron densities, vibrational normal modes, various kinds of spectra, and many other properties. **QC-Lab** can accommodate density functional and wave function-based electronic structure theories, as well as semiempirical calculations based on methods like PM3. The **CNDO/INDO** and **UV-Spec** codes provide additional functionality for doing semiempirical calculations based on methods like INDO/S that are relevant to the determination of electronic spectra.



We have developed five assignments in which students can use various components of **NUITNS** in applications that show the capabilities, and occasionally failures, of quantum mechanics to describe real-world problems. These include:

a) The thermodynamics and thermochemistry associated with methanol, including studies of solvation effects and combustion modeling,

b) The optical and chemical properties of doped nanodiamonds (substitutional and endohedral doping effects for diamondoid structures)

c) Retinal isomerization (calculating isomerization energies for chomophores involved in vision),

d) The structures and optical properties of silver nanoparticles (calculating electronic spectra of gold clusters as models of nanoparticles),

e) Carbon nanotube mechanical properties (determining stress-strain behavior of individual carbon nanotubes).

The first two of these assignments are described in a paper by T. Simeon, C. Aikens, B. Tejerina and G. C. Schatz (*J. Chem. Ed", submitted, 2010'). The other three assignments are*

presented in files that are linked below. These assignments provide opportunities for the students to gain experience in building molecules, testing different electronic structure models and basis sets, calculating thermodynamic, mechanical and spectroscopic properties, making comparisons with experiment, and ultimately to assess the quality of the results.

Links to other documents:

1. Retinal isomerization project
2. Au nanoparticle spectrum project
3. Carbon nanotube mechanical property project