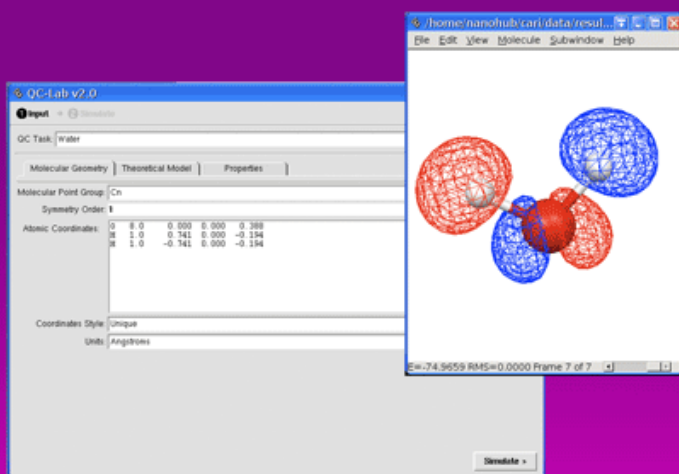
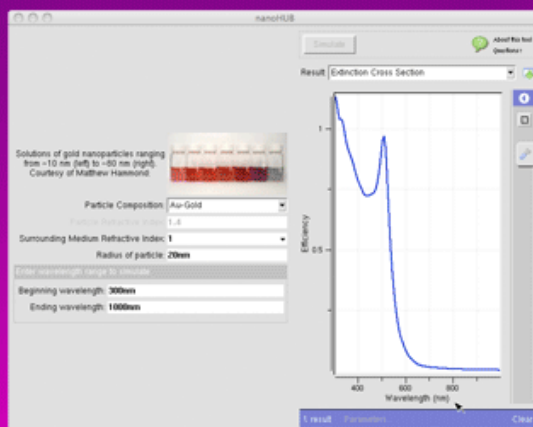


General Chemistry. Nanoscience and Computational Chemistry Modules

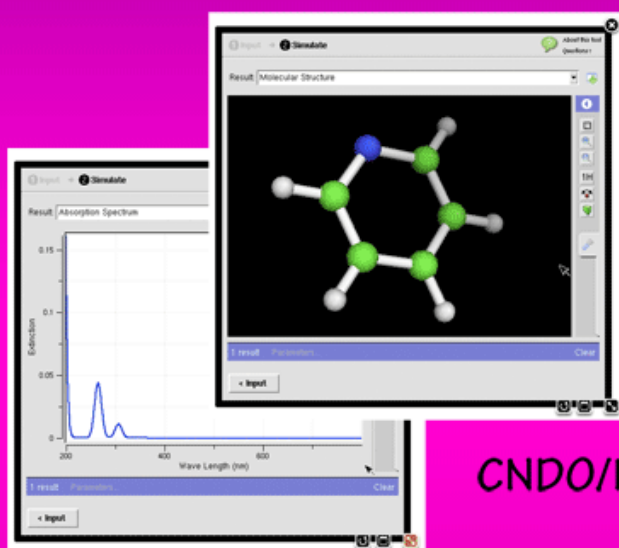
General Chemistry Tools



QC-Lab



Nanosphere Optics Lab



CNDO/INDO



General Chemistry courses are taught at every college and university, and usually the goal is to cover the field of chemistry broadly over the course of an academic year. The topics included in such courses have evolved with time, but generally the emphasis is on the structural and thermodynamic properties of atoms and molecules and on chemical reactions and kinetics. New topics which have gradually appeared in the last 20 years are biomolecules and the properties of materials. Topics which usually don't get much attention in General Chemistry textbooks are nanomaterials and computation.

At Northwestern University, we have been adding new material pertaining to nanomaterials and computation to our General Chemistry classes since 2006. The new material has been added as modules into the laboratory component of the course, and includes experiments in which the students synthesize nanoparticles, measure some properties, and then use codes on nanoHUB to model the results and interpret the experiments.

In addition, we have developed a computational chemistry lab that is a stand-alone one-week assignment for General Chemistry lab. These laboratory modules are coordinated with lecture material in the General Chemistry courses, either in conjunction with the descriptive chemistry section or when we talk about quantum mechanics. During the last several years, these modules have been used in classes where hundreds of students use nanoHUB at the same time.

We have developed three modules. Writeups for the three labs are available as nanoHUB resources or as a document attached to this page. These write-ups include experimental procedures as well as computational modeling. Obviously the ability to do the experiments depends on what you have in your chemistry lab!

[Gold and silver nanoparticle synthesis, characterization and modeling](#)

This is a combined experiment/computational lab in which gold nanoparticles are synthesized, their optical properties are measured, and then a nanohub tool named the [Nanosphere Optics Lab](#) is used to model these optical properties and derive information from the observed spectra.

Cadmium selenide synthesis, characterization and modeling

[CdSe quantum dot module.pdf](#) (902 KB, uploaded by Marcelo Carignano 7 years 5 months ago)

by Evan R. Trivedi and Shelby L. Hatch, Department of Chemistry, Northwestern University, Evanston, IL 60208

This is a combined experiment/computational lab in which cadmium selenide quantum dot nanoparticles are synthesized, their spectra are studied, and the results are modeling using the [CNDO/INDO](#) semiempirical electronic structure code. Synthesis and Size Dependent Properties of CdSe Quantum Dots

[Electronic structure calculations using QC-Lab](#)

This is a purely computational project that is concerned with using the nanohub tool [QC-Lab](#) to create and optimize molecules, and to study their spectroscopic and structural properties. The

molecules studied are generally small molecules of interest to atmospheric chemistry, however the tool can be used for applications in nanoscience, and there are followup projects (not appropriate for freshman) that study the properties of carbon nanotubes and molecules important in vision.

These laboratories use three applications on nanoHUB:

[Nanosphere Optics Lab](#)

This code performs Mie theory calculations to determine the extinction and scattering spectra of spherical nanoparticles.

[CNDO/INDO](#)

This code performs semiempirical electronic structure calculations and is intended to be used to model electronic spectra.

[QC-Lab](#)

This code is a general purpose interface for the GAMESS electronic structure code, and can be used to determine the structures and spectra of molecules and materials based on density functional, semiempirical and wave-function-based methods.

[NUITNS](#)

NUITNS is an umbrella for several codes that can be used for teaching nanoscience, including QC-Lab and INDO/CNDO. These codes can be launched from within NUITNS or run stand-alone.