Version April 23, 2010

Computational Chemistry Focus Area

Description

Computational chemistry is, in its broadest sense, the application of computers to understand, interpret and predict chemical phenomena, i.e. the behavior and properties of atoms, molecules and solids. Due to ongoing advances in computer hardware and software, computational chemistry has developed into an indispensible tool for, and a major branch of modern chemistry. Computational chemistry methods range from those based on rigorous quantum chemistry ("ab initio" methods) to "semi-empirical" methods that use empirical (experimental) data as input, to "molecular mechanics" methods that apply classical physics, and even to "black-box" methods (QSPR) that rely on statistical correlations without detailed physical models. Computational chemists develop new algorithms, implement them into efficient computer programs, and use computational chemistry methods to solve chemical problems. The application and, in particular, the development of new computational chemistry methods requires an understanding of the underlying physical and mathematical methods and models, as well as a good working knowledge of relevant principles in computer science. Computational chemists find jobs in the pharmaceutical industry (drug design), in the chemical industry (catalyst modeling), and even in financial institutions ("if you can model chemistry, you can model the financial markets").

Non-chemistry courses

At least 3 out of:

COMP2160, COMP2190,
MATH2300, MATH2600
PHYS3680, PHYS3650

Chemistry courses

2nd year: CHEM2290 or CHEM3570

… in addition to any prerequisites, of course.

3rd and 4th years:

CHEM3360
CHEM4660 *(Computational chemistry, formerly numbered as CHEM4650)*

At least 2 out of:

CHEM3370
CHEM3580
CHEM4640
CHEM4670

Two further courses at the 3000/4000 levels