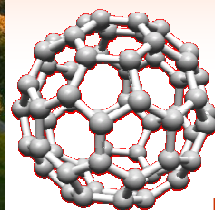


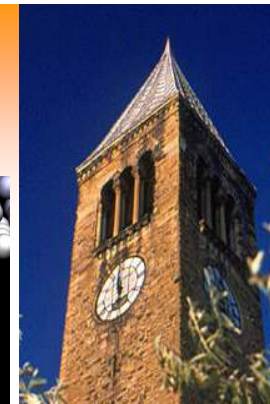
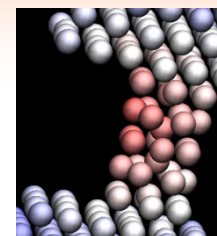


2010 Joint NNIN/C & NCN Fall Workshop

Building a Collaborative Framework for Nanoscale Simulations



November 14th-16th, 2010
Cornell University, Ithaca, NY



http://www.cnf.cornell.edu/cnf_fallworkshop2010.html

Overview: Nanoscience relies on intensive atomistic simulations that generate copious amounts of data. Since various ab-initio and empirical approaches exist in the field, there is a growing need to develop a *common collaborative framework* for meaningful comparisons between calculations and to also provide a set of robust technical components and results for the next generation of researchers.

This workshop brings together leading figures in fields of materials and nanostructure simulation to help develop a set of *lingua franca* formats & libraries for easy translation of input and output files between codes. We will address the creation of international cyberinfrastructure resources that deliver trusted components for atomistic calculations such as empirical potentials, pseudopotentials, basis sets, and atomic coordinates.

Confirmed Speakers:

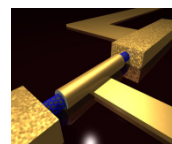
Gerhard Klimeck (Purdue) Jim Sethna (Cornell)
Geoffrey Hutchison (Pittsburgh) Derek Warner (Cornell)
Matthieu Verstraete (University of Liege, Belgium)
Karsten Jacobsen (Technical University of Denmark)
Derek Stewart (Cornell)

Registration Deadline:

November 3, 2010

Seating is limited to 40 participants

Organizer: Derek Stewart (stewart@cnf.cornell.edu)

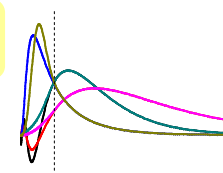


Photograph by Zack Schildhorn

Workshop Topics

Trusted Components for Calculations

- Pseudopotentials Basis Sets
- Empirical Potentials Crystallographic Data



Standing on the Shoulders of Giants

- Developing a Database of Input Files based on Previous Research
- Common IO Formats & Libraries for Ab-initio Calculations

Overview of Current Efforts in the Field Including...

- Atomic Simulation Environment NCN Nanohub
- OpenBabel NNIN Virtual Vault
- European Theoretical Spectroscopy Facility (ETSF) DFT Libraries

Fully Reproducible Science

- Linking Calculations directly with Publications
- Input Files as a part of Article Supplementary Info

Tutorial Sessions on ASE, Abinit, NEMO, and more!

