Cornell Department of Materials Science and Engineering

Faculty

- 16 FTE

Undergraduate Students

- Average class size of **35 students** (fluctuations from 25 to 60)
- About 50% of undergraduates join a research group and perform research during junior and senior year (senior thesis)
- 50% go to graduate/professional schools
- 50% industry and research labs

Graduate Students and postdocs

- About 70 graduate students
- About 30 postdocs and visiting researchers

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Materials Science and Engineering at Cornell

Common Engineering Curriculum (Years 1 and 2)

- 4 Math, 1 Chemistry, 3 Physics, 2 Computer Science courses, ...

Introductory courses

- Y2 Fall Mechanical Properties
- Y2 Spring Electronic Materials for the Information Age

Structure

- Y2 Spring Structure of Matter
- Y3 Fall Thermodynamics
- Y3 Spring Kinetics

Properties

- Y3 Fall Chemistry of Materials
- Y3 Spring Electronic and Magnetic Properties
- Y4 Fall Mechanical Properties of Materials

Junior and Senior Lab

Junior and Senior Design Course

Electives: Materials, Materials Applications Outside Technical

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Computational Materials Science at Cornell

Common Engineering Curriculum

- **2 Computer Science course**

Introduction to Computing Using MATLAB

Programming and problem solving using MATLAB. Emphasizes the systematic development of algorithms and programs.

Transition to Object-Oriented Programming

Introduction to object-oriented concepts using Java.

4 Math courses, MSE core courses:

- Use Matlab or Java in homework assignments

Elective course: Computational Materials Science (2 lectures, 1 lab per week)

Introduction to state-of-the-art comput[illegible] emphasis on the atomic and nano scal[illegible] supercomputers. Enrollment: about 15

Other elective courses:
Finite element methods (MAE, TAM)
Parallel programming (CEE, CIS)
Density functional methods (Physics)

Junior and Senior Lab: Statistical me[illegible]

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Computational Materials Science Course

Elective course: Computational Materials Science (2 lectures, 1 lab per week)

Introduction to state-of-the-art computational methods in materials research with emphasis on the atomic and nano scales and hands-on modeling using PCs and supercomputers. Enrollment: about 15 juniors and seniors, 5 graduate students

Lectures

- Interatomic force fields and molecular mechanics methods
- Quantum mechanical methods: HF, quantum chemistry and DFT
- Practical aspects of DFT calculations
- Finite temperature effects: Excitations in materials and how to sample them
- Molecular dynamics and Monte Carlo methods
- Transition state theory and infrequent event methods

Labs

- Supercomputers, Linux, batch environment at the CNF cluster
- Defect formation energies and surface energies using interatomic potentials and the **GULP** code
- Ground states, excited state and reaction energies for molecular systems using quantum chemistry with **NWChem** and **Avogadro** for visualization
- Equation of state and the electronic structure of semiconductors using the DFT package **PWSCF**
- Solid/liquid phase transformations, diffusion and vibrational properties using **LAMMPS** MD code

Project

- Develop a program to model materials or use existing software to calculate materials properties

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Student Projects

Students (1) propose a project and write a proposal
(2) Perform the simulations on supercomputers or write the code
(3) Present the project to the class (20 minute presentation)
(4) Write up a project report.

Material	Method	Software
Conducting polymers: Polypyrrole derivatives	DFT-B3LYP, geometry, HOMO-LUMO	Gaussian03
FeS and elemental S under pressure	DFT, E(V), random searches	VASP
Gratzel cell dye: Coumarin 343 on NiO	DFT-B3LYP, geometry, HOMO-LUMO	Gaussian03
Adsorption of small molecules on PtPb	DFT, geometry optimization, energies	VASP
Amorphous binary oxides TaGeO as dielectric	DFT-B3LYP, geometry, polarization	Gaussian03
Graphene single and bilayer	AI-REBO potential	LAMMPS
Boiling point of hydroflouroethers	Empirical potentials	DL-POLY
Solute stabilization of Ti alloys	DFT	VASP
Photonic bandgaps	Maxwell's equation	MIT Photonic band (MPB)
Edge and screw dislocations in fcc or bcc metals	Empirical potentials	MD++ and AtomEye
Stacking interactions in DNA	DFT+vdW or MP2	Gaussian03
High-pressure methane	Empirical potentials (AI-REBO)	LAMMPS
Vacancy diffusion in Ge nanocrystals	DFT+NEB	Siesta

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Software

Only use software that is either freely available or has a site license so students can use it in their research and other classes

- MD: LAMMPS, Gulp
- DFT: PWSCF
- Quantum Chemistry: NWChem, Gaussian09
- Photonics: MIT Photonic Bands
- Visualization and structure generation: Avogadro, wxDragon, GaussView, AtomEye