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
# 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
### Computational Materials Science at Cornell

#### Common Engineering Curriculum
- 2 Computer Science course

<table>
<thead>
<tr>
<th>Introduction to Computing Using MATLAB</th>
<th>Transition to Object-Oriented Programming</th>
</tr>
</thead>
<tbody>
<tr>
<td>Programming and problem solving using MATLAB. Emphasizes the systematic development of algorithms and programs.</td>
<td>Introduction to object-oriented concepts using Java.</td>
</tr>
</tbody>
</table>

#### 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 computational methods, with emphasis on the atomic and nano scales using PCs and supercomputers. Enrollment: about 15 students.

#### Junior and Senior Lab: Statistical methods and data analysis

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

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