**Atom-based computational methods for materials**

Evan Reed, Spring Quarter 2014

**Graduate level course:**
Introduction to atom-based computational methods for materials with primary emphasis on quantum methods. Density functional theory with periodic boundary conditions. Analytical interatomic potentials and their construction. Computation of mechanical, optical, electronic, vibrational properties of bulk materials and nanomaterials. Molecular dynamics and Monte Carlo methods with applications to structure searches and transport properties. Homeworks involve implementation and use of these algorithms in both MATLAB and research level codes.

**Prerequisite:** Undergraduate level quantum mechanics

**Syllabus:**

**Empirical atomic potentials:**
- Construction of an inter-atomic potential
    - Two-body
    - Many-body
- Lennard-Jones, Stillinger-Weber, REBO, EAM, MEAM, et al.
- Successes and failures

**Total energy calculations**
- Periodic and other boundary conditions
- Energy minimization methods
    - Steepest descent
    - Conjugate gradients
    - Simulated annealing
- Metastability
- High pressure and enthalpy
- Structure prediction
- Lennard-Jones vacancy energy

**Statistical and time-domain methods**
- Molecular dynamics and integration algorithms
- Thermostats, constraints, boundary conditions
- Non-equilibrium systems
- Transport and fluctuation-dissipation theorem
- Vibrational properties
- Monte Carlo
- Structure searches
- Free energy, quantum nuclear effects

**Density functional theory**
- Hartree, Hartree-fock, electron correlation
- Practical DFT, approximations, limitations
- Exchange-correlation functionals, range-limited, van der Waals
- Basis sets

- Pseudopotentials – make a pseudopotential
- Energy minimization, forces
- Brillouin zone, Bloch's theorem
- Band structure, electronic properties
- Time-dependent DFT, optical properties, GW/BSE

**DFT Applications**

- Graphene band structure and adatom adsorption
- Elastic moduli
- Phase diagrams, transformations

**Homework topics:**

**HW 1:** Analytic interatomic potentials
**HW 2:** Make a MATLAB code for vacancy calculations with periodic boundary conditions
**HW 3:** Make a MATLAB code for Molecular Dynamics (Lennard-Jones); diffusion; crystal/liquid
**HW 4:** Make a MATLAB code for Monte Carlo; Simulated annealing
**HW 5:** Make a MATLAB single particle bands code for hydrogen atom and lithium crystal; Quantum Espresso DFT calculations of Si elastic moduli
**HW 6:** Make a lithium pseudopotential with a MATLAB code; DFT with Quantum Espresso: graphene chemistry and bands, graphane formation energy