MS/ME/PY/CH 508: Computational Methods in Materials Science, Spring 2011

Instructor:
Professor Xi Lin
Department of Mechanical Engineering and Division of Materials Science and Engineering
Rm. 207, 15 Saint Mary's Street
Brookline, MA 02446
Phone: (617) 358-3417
Email: linx@bu.edu
Course page: http://oned.bu.edu/MS508

Lectures: MW 2-4 PM at LSEB B03
Office hours: MW 4-5 PM; email linx@bu.edu for additional appointments

Lecture notes: http://oned.bu.edu/MS508/lecture.html

Textbooks:

1) A Guide to Feynman Diagrams in the Many-Body Problem, by Richard D. Mattuck (1976) ISBN 0-486-67047-3
2) Electronic Structure: Basic Theory and Practical Methods, by Richard M. Martin (2003) ISBN: 0-521-78285-6
3) Computer Simulation of Liquids, by M. P. Allen and D. J. Tildesley (1989) ISBN: 0-19-855645-4
4) Simulating the Physical World, by Herman J. C. Berendsen (2007) ISBN: 0-521-83527-5

References:

1) Handbook of Materials Modeling, edited by Sidney Yip (2005) ISBN 1402032870
2) Numerical Recipes: The Art of Scientific Computing, by William H. Press, Saul A. Teukolsky, William T. Vetterling, and Brian P. Flannery (2007) ISBN: 978-0-521-88068-8

Pre-requisites by Topic: Quantum mechanics, statistical mechanics, and solid state theory; or consent of instructor.

Goals: To apprehend core knowledge of materials theory and to gain hand-on experience of performing predictive materials modeling and simulation

Grading:
Five assignments (30%): the best three count
Quizzes (40%): every lecture
Individual final project (30%)

Assignments: Homework announcements will be communicated through the course page at http://oned.bu.edu/MS508. Homework assignments are due a week after they are handed out.

Lecture Schedule:

Lecture (week)	Topic	Textbook
1	Introduction - Materials theory - Computational materials science Many-body problem - Quasi-particle	T1 and R1
2 3 4 5 6 7	Electronic structure - Green's function propagator - Second quantization - Feynman diagram - Dyson's equation - Adiabatic approximation - First-order processes -- Forward scattering: Hartree -- Forward and exchange scatterings: Hartree-Fock - Dynamical screening -- Random phase approximation -- Configurational interaction -- Perturbation -- Coupled cluster * Computational lab I - Quantum Monte Carlo -- Green's function Monte Carlo -- Short-time approximation - Density functional theory -- Universal functional -- Density matrix -- Exchange-correlation functional -- Pseudopotential - Tight-binding * Computational lab II	T1, T2, and T4 R1 and R2 Papers
8 9	Ensemble Fluctuation-dissipation theorem Partition function Time-correlation function Molecular dynamics Stochastic processes * Computational lab III	T3 and T4 R1 and R2 Papers
10	Coarse graining Fluid dynamics Mesoscopic continuum dynamics Percolation theory	T4 R1 and R2 Papers
11	Materials defect theory - Topological defects	Papers

12	- Self-assembly - Complex fluids -- Polymers and bio-polymers --- Protein: ion channel --- DNA: small polaron Scaling theory - Renormalization group theory - Anderson localization Dimensionality - 1D, 2D, 3D, and fractal dimensions	
13	Final project presentation	