EMA 6803 Classical Methods in Computational Materials Science

1. Catalog Description (3 hours): Proficiency developing and using common tools for computational materials research at the atomic level.
2. Pre-requisites and Co-requisites: Experience with UNIX; knowledge of programming with FORTRAN, C++, or other technical programming language; familiarity with the fundamentals of the structure of materials, including metals, ceramics, and polymers; and the consent of instructor.
3. Course Objectives: To train students in the application of classical, atomic-scale methods and first-principles, density functional theory (DFT) to problems in materials science. This includes learning about the theoretical underpinnings of the methods used, writing classical molecular dynamics programs from scratch, and learning to use DFT software packages.
4. Instructor: Dr. Susan Sinnott
    a. Office: 154 Rhines Hall
    b. Telephone: 352-846-3778
    c. E-mail address: sinnott@ufl.edu
    d. Class Web site: None
    e. Office hours: Tuesday: 9:30-10:30, Thursday: 10:30-11:30
5. Meeting Times: Tuesday 2nd period, Thursday, 2nd and 3rd periods
6. Meeting Location: MAEB 238
7. Textbooks and Software Required:
    a. Title: Computer Simulation of Liquids
    b. Authors: M.P. Allen and D.J. Tildesley
    c. Publication date and edition: 1987, 1st
    d. ISBN number: 198556454

    a. Title: Interatomic Forces in Condensed Matter
    b. Author: Mike Finnis
    c. Publication date and edition: 2010, 1st
    d. ISBN number: 9780199588121

    Students will make use of student accounts on the University of Florida High Performance Computing Cluster (HPC) (http://www.hpc.ufl.edu/). Students may already have accounts that are sponsored by their research adviser but the resources of the research group should not be impacted by course-related activities. Rather, students should request a separate account for course assignments and projects. This will ensure correct resource allocation and accounting. Class accounts will be deleted two weeks following the end of the semester. The class as a whole is limited to 32 CPU cores simultaneously at any given time. All class accounts will be deleted two weeks after the end of the course and permissions to use licensed software will expire at that time.
8. Course Outline:

Date (#periods)	**Topics**	**Book (pages)**
8/22 (2)	Introduction to the course Equations of motion, finite difference methods	#1 (71-84)

8/27 (1)	Molecular dynamics of rigid non-spherical bodies	#1 (84-109)
8/29 (2)	Examples and additional methods	Literature
9/3 (1)	**HPC orientation session**	
9/5 (2)	Heart of the matter, neighbor lists, multiple time-step methods	#1 (140-152)
9/10 (1)	Long-range forces, dust	#1 (152-168)
9/12 (2)	Starting up, organization, estimating errors	#1 (168-181, 191-196)
9/17 (1)	*Sinnott travel: Brookhaven site visit* (Make-up class: Beyond standard MD)	Literature
9/19 (2)	*Sinnott travel: Brookhaven site visit* **VASP instructional session**	
9/24 (1)	Time-independent Schrodinger equation, wave mechanics, basis vectors	#2 (3-20)
9/26 (2)	**Individual reports due, group presentations**	
10/1 (1)	Periodic boundary conditions, local orbitals, spherical harmonics	#2 (20-37)
10/3 (2)	Variational Principle, Schrodinger equation, density matrix, DOS, jellium	#2 (37-55)
10/8 (1)	*Sinnott travel: KS EPSCoR conference* (Make-up class: Matrix eigenvalue problem and pseudopotentials)	#2 (55-63)
10/10 (2)	Functionals, derivatives, and Thomas-Fermi	#2 (64-70)
10/15 (1)	Kohn-Sham equations	#2 (70-78)
10/17 (2)	Hellmann-Feynman theorem, perturbation theory	#2 (79-87)
10/22 (1)	*Sinnott travel: CALD all hands meeting* (Make-up class: Recent progress in DFT methods)	Literature
10/24 (2)	**Individual reports due, group presentations**	
10/29 (1)	*Sinnott travel: AVS*	
10/31 (2)	*Sinnott travel: AVS*	
11/5 (1)	Tight-binding and the tight-binding bond model	#2 (192-194, 200-207)
11/7 (2)	Moments of the DOS, recursion, second-moment approximation	#2 (218-237)
11/12 (1)	Fourth-moment approximations, bond-order potentials	#2 (237-252) + literature
11/14 (2)	Embedded Atom Method (EAM) and related potentials, ionic potentials	#2 (253-274) + literature
11/19 (1)	Recent progress in interatomic potentials	Literature
11/21 (2)	**Individual reports due, individual presentations start**	

11/26 (1)	**Individual presentations conclude**	
12/3 (1)	*Sinnott Travel: Fall MRS* **Software project due** Course evaluation due (electronic)	

9. Attendance and Expectations: Class participation and discussion in class is part of the course grade, so attendance is highly encouraged.
10. Grading:

Class attendance and informal discussion	15%	
Individual software project	15%	write MD software from scratch
Group oral presentations	20%	15-minute presentations
Individual oral presentations	25%	7-minute presentation
Individual written reports	25%	7-page written report

11. Grading Scale: Grades will be curved and the final letter graded determined by the instructor.

Graduate students need an overall GPA of 3.00 truncated and a 3.00 truncated GPA in their major (and in the minor, if a minor is declared) at graduation. For more information on grades and grading policies, please visit:
http://gradcatalog.ufl.edu/content.php?catoid=4&navoid=907#grades

12. Honesty Policy – UF students are bound by The Honor Pledge which states, "We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code. On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied: "On my honor, I have neither given nor received unauthorized aid in doing this assignment." The Honor Code (http://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class.
    Note that failure to comply with this commitment will result in disciplinary action compliant with the UF Student Honor Code Procedures.
    See http://www.dso.ufl.edu/sccr/procedures/honorcode.php
13. Accommodation for Students with Disabilities – Students Requesting classroom accommodation must first register with the Dean of Students Office. That office will provide the student with documentation that he/she must provide to the course instructor when requesting accommodation.
14. UF Counseling Services –Resources are available on-campus for students having personal problems or lacking clear career and academic goals. The resources include:
    - UF Counseling & Wellness Center, 3190 Radio Rd, 392-1575, http://www.counseling.ufl.edu/cwc/Default.aspx, counseling services and mental health services.
    - Career Resource Center, Reitz Union, 392-1601, career and job search services.

    University Police Department 392-1111
15. Software Use – All faculty, staff and student of the University are required and expected to obey the laws and legal agreements governing software use. Failure to do

so can lead to monetary damages and/or criminal penalties for the individual violator. Because such violations are also against University policies and rules, disciplinary action will be taken as appropriate. We, the members of the University of Florida community, pledge to uphold ourselves and our peers to the highest standards of honesty and integrity.

16. Students are expected to provide feedback on the quality of instruction in this course based on 10 criteria. These evaluations are conducted online at https://evaluations.ufl.edu. Evaluations are typically open during the last two or three weeks of the semester, but students will be given specific times when they are open. Summary results of these assessments are available to students at https://evaluations.ufl.edu/results. “