PHY5937 009, PHY 4936 009: Practical Guide to Density Functional Theory Computations (Spring 2021)

Instructor: Dr. Inna Ponomareva; Office: ISA 5103; E-mail: iponomar@usf.edu; telephone: 974-7286

Texts: 1. Density functional theory: a practical introduction by David S. Sholl and Janice A. Steckel (USF electronic resource, free to USF students); 2. Atomic and Electronic Structure of Solids by Kaxiras, Efthimios (USF electronic resource, free to USF students); 3. The ABC of DFT by Kieron Burke (free to download from https://dft.uci.edu/research.php#theabcofdft)

Other required resources: 4. Hack Your Brain: Secrets of an Elite Manhattan Tutor, by Elie Venezky and Patrycja Slawuta; 5. computer/laptop with internet connection.

Class: TR 11:00am-12:15pm ISA 4010

Office Hours: TR 2:00pm-3:00pm and by appointment.

Prerequisites: Quantum Mechanics at the undergrad level or higher or some sorts of exposure to Quantum Mechanics.

Course Outline and Objectives: In 1998 Walter Kohn shared the Nobel Prize in Chemistry for his development of the density-functional theory (DFT). Since then DFT became the standard tool for quantum-mechanical level of modeling in physics, chemistry, materials science and many areas of engineering. This is a "crash course" practical introduction to the basics of DFT that does not require any prior background in solid state physics or computations. The goal is to develop basic but solid and conceptualized understanding of DFT computations and its foundations through an integrated theory/practice approach. The free software, Quantum Espresso, will be used for DFT computations which will be executed on USF supercomputer. For each Chapter homework will be assigned and due at the beginning of the next Chapter. Examples of topics are structural optimization, calculations of vibrational frequencies, equilibrium phase diagrams, electronic structure and magnetic properties.

This is an experimental class that integrates strategies of efficient learning. Students will learn and implement effective and proven strategies to develop into an efficient, successful learner and take full advantage of their brain. The expectation is that these skills will propel students' success in this and other courses. An extra credit in the form of one grade increment may be offered for class attendance and participations. Students must attend 24 out 30 classes to qualify. This could modify if class schedule or form of instructions change considerably.

Course Grading Breakout		
	Homework	80 %
	Mid-term Exam	10 %
	Final	10 %

Course Grading

> 93		A
90	< 93	A-
87	< 90	B+
84	< 87	B
80	< 84	B-
77	< 80	C+
74	< 77	C
70	< 74	C-
67	< 70	D+
64	< 67	D
60	< 64	D-
	< 60	F

Tentative Schedule and Examination Dates

Week Beginning	Topics (Chapters in Text 1, Chapters in Text 2, Chapters in Text 4)
Jan 10	Intro to crystalline solids, basic of linux, submitting jobs on a supercomputer (1, Module I-II)
Jan 17	Intro to DFT (1, 2, Module III-IV)
Jan 24	
Jan 31	Setting up DFT calculations for Simple Solids (2, 1, Module V)
Feb 7	Basic DFT calculations: energy cutoff, k-point mesh, optimization (3,3, Module VI-VII)
Feb 14	
Feb 21	Electronic Structure and Magnetic Properties (8,4-5,7, Module VIII)
Feb 28	Midterm March 4th
Mar 7	DFT calculations for Surfaces and Solids (4, 11)
Mar 14	DFT calculations of vibrational frequencies (5, 6)
Mar 21	
Mar 28	Computations using Transition State Theory (6)
Apr 4	
Apr 11	Spring Break
Apr 18	Equilibrium Phase Diagrams (7)
Apr 25	Ab Initio Molecular Dynamics (9), Beyond Standard calculations (10)
May 2	FINAL tentatively on Thursday, May 6th

NOTE

Students who anticipate being absent from exams due to a major religious observance must provide notice of the date(s) and event(s) to the instructor, in writing, by the second class meeting. Any student with a disability is encouraged to meet with me privately during the first week of class to discuss accommodations. Each student must bring a current Memorandum of Accommodations from the Office of Student Disability Services (974-4309, SVC1133) which is prerequisite for receiving accommodations. Accommodated examinations through the Office of Student Disability Services require at least two weeks notice.

COVID-19

If USF goes online due to pandemic the course will be instructed online. Students need to have electronic device with webcamera and microphone and are expected to appear for on-line classes at regular times. The exams will be proctored using Proctorio software.

Covid-19 Procedures

All students must comply with university policies and posted signs regarding COVID-19 mitigation measures, including wearing face coverings and maintaining social distancing during in-person classes. Failure to do so may result in dismissal from class, referral to the Office of Student Conduct and Ethical Development, and possible removal from campus.

Additional details are available on the University's Core Syllabus Policy Statements page: https://www.usf.edu/provost/faculty/core-syllabus-policy-statements.aspx