

Instructor: Douglas L. Irving, 3028D Engineering Building I, Phone: (919) 515-6154, E-Mail: ddirving at ncsu.edu

Office Hours: Tuesday, 3:00-4:00 PM (zoom)

Suggested Textbooks: (These texts are a starting point and will be supplemented by handouts, articles, and lecture notes. Digital versions of these texts are available from the library.)

1. *Density Functional Theory: A Practical Introduction* by David S. Sholl and Janice A. Steckel
2. *Materials Modelling using Density Functional Theory: Properties and Predictions* by Feliciano Giustino
3. *Electronic Structure: Basic Theory and Practical Methods* by Richard M. Martin

Course Outline: The course will be broken into three parts, 28 lectures. These parts are listed below with key subjects that will be addressed. This list is not comprehensive.

1. Theoretical background (4-5 Lectures)
 - Common units
 - Electrostatics
 - Potential energy
 - Poisson Equation
 - The Schrödinger equation
 - The first real solution: The infinite square well
 - Common problems solved in an introductory quantum class
 - Variational principle and solutions
2. Density functional theory and its implementation (12-14 Lectures)
 - Theory of DFT
 - Mathematical considerations
 - Numerical solution of the Poisson equation
 - Ewald approximation
 - Setup and solution of the Kohn-Sham equations
 - The Hartree potential
 - Basis set up
 - Iterative solutions
 - Quantum dot

- Hydrogen molecule
 - Pseudopotentials, computational efficiency, and solids (MAYBE)
3. Application of DFT to materials related problems using an established DFT code. This includes the following and possibly more. (10-11 Lectures)
- Implementation of DFT in available codes
 - Basis set convergence
 - Equation of state
 - Band structure and density of states
 - Vibrational properties
 - Surface energies
 - Minimum energy pathways for surface diffusion

Grade Policy: The final grade for the course will be based on the results of assignments within each section of the course described above. The assignments in the Theoretical background section will count for 25% of the final grade. The work in the Theory of DFT and the Practical applications of DFT to MSE will count towards 35% and 35% of the final grade, respectively. There will also be a participation grade of 5%. This comes in the form of turning in a short summary of lecture material each week. Assignments will be graded on a blend of completeness and correctness. This will be clearly stated based on each assignment. Course grades will be assigned following the usual 10 points per letter grade. Plus and minus grades (e.g., A+, A, A-) will be assigned per the convention 90-92.9 = A-, 93-97.9 = A, 98-100 = A+.

Assignment policies: The work you turn in is expected to be your own and you should abide by the university's academic integrity policy (discussed below). You must work on the assignments yourself, but formation of study groups is encouraged. Appropriate discussion about an assignment includes discussing the interpretation of the problem statement, sharing ideas or approaches for solving the problem, and explaining concepts involved in the problem. Any other aid would be unauthorized and a violation of the academic integrity policy. Unauthorized aid additionally includes accessing online solutions, sharing your solutions with others, and walking others through each step of a problem. None of the assignments should be posted to online websites (i.e. CourseHero). The instructor reserves copyright on the material of the class. You are allowed to use and retain this for your own personal use you require instructor permission for distribution outside of the class.

Assignments: Assignments will be typically made available 1-1.5 weeks in advance and in some instances longer. All of the assignment problems will be graded for completeness, and most will be graded for correctness. You do not need to wait until the deadline to turn in assignments. Final versions of assignments will be uploaded to Moodle for grading unless otherwise specified. The format of what is to be turned in will be specified with each assignment and these instructions are expected to be followed. Late assignments will not be accepted without prior approval. Approval of late work will only be given for extenuating situations.

CAUTION: Do not wait to do your assignments on the due date, start earlier. Some of this course involves simulation (which can crash and not run) and building programs (which rarely works the

first time). While crashes and programming bugs are frustrating, they are part of learning. Trying to fit them into a fixed window of time increases the pressure and lowers your ability to learn the subject.

Course Objectives: The objectives of this course are for the student to learn the fundamentals of the electronic structure problem, how this problem can be solved through implementation of a density functional theory, and how to implement a plane-wave pseudopotential code to solve standard problems faced in Materials Science and Engineering. The course begins by providing a necessary background in electrostatics, quantum mechanics, and the variational solutions of the Schrödinger Equation. Challenges associated with the solution of the many electron and means to overcome these obstacles by use of DFT will be discussed. Students will also be given an overview of materials properties that can be calculated within DFT followed by exercises that illustrate of how this is implemented in a plane-wave code.

Technology Requirements: Some homework problems will require use of Mathematica, Maple, Wolfram Alpha or equivalent mathematical computing software, which are available to students for free through the NCSU software website. This course also uses Moodle Office hours are through Zoom. Recordings of lectures may also be made available through Panopto, but the default mode of course delivery is in-person only. For later sections of the class, we will build a version of DFT using Python3, Numpy, and Scipy. I use Conda for environment management but this is not required. Finally, a computer will be used to access the NCSU HPC for the final part of the class.

Academic Honesty: You are responsible to the NCSU student code of conduct:

<http://policies.ncsu.edu/policy/pol-11-35-01>

DISCLAIMER Information in this syllabus is subject to minor changes and the possession of it does not ensure that you have all the correct information required to successfully complete the semester. Announcements of changes will be made and students are responsible for obtaining additional information by attending class, watching class videos, and staying up to date on class announcements.

Requirements for Credit-Only Grading (S/U): In order to receive a grade of S, students are required to complete all assignments, and earn a grade of C- or better. Conversion from letter grading to credit only (S/U) grading is subject to university deadlines. Refer to the Registration and Records calendar for the deadlines. For more details refer to:

<http://policies.ncsu.edu/regulation/reg-02-20-15>

Incomplete Grades (IN): Incomplete grades will be given only under extenuating circumstances, in accordance with NCSU policy as described at the website below. The burden of fulfilling an incomplete grade is the responsibility of the student.

<http://policies.ncsu.edu/regulation/reg-02-50-03>

University Policies: All NC State University policies can be found at the following web page:

<http://policies.ncsu.edu/policy/>

Three of these policies are reprinted for your convenience:

Academic Integrity: As a student enrolled in this class, you are expected to honor the NCSU policies regarding academic integrity found in the Code of Student Conduct at:

<http://policies.ncsu.edu/policy/pol-11-35-01>

In this course, this policy applies primarily to cheating on assignments, which will not be tolerated. See the Assignments section for a discussion of what is allowed and disallowed. Evidence of cheating on assignments and all cases of academic misconduct will be submitted to the Office of Student Conduct. Students found guilty of academic misconduct will be subject to, at a minimum, a zero on the assignment in question, up to a zero for that course component (e.g., a zero for the homework portion of the final grade), or a failing grade in the course, depending on the nature of the violation. In addition, if you are found guilty of academic misconduct in the course, you will be on academic integrity probation for the remainder of your years at NCSU, may be required to report your violation on future professional school applications, and could have further implications for ROTC positions and/or employment on campus, including University Housing. It's not worth it!

If there are questions regarding any matter relating to the standards of academic integrity in this course or on a given assignment, they should be discussed with the instructor prior to doing any work. If any violation of the academic integrity policies is observed, please notify the instructor immediately.

The documents – lecture videos and electronic copies of homework assignments and solutions, exams and solutions, and handouts – made available to you for this course are intended only for your personal use. You are not allowed to share any content of the class with any person not signed up for the course this semester; a personal, public, or commercial website; or any other news or advertising media.

Students with Disabilities: Reasonable accommodations will be made for students with verifiable disabilities. In order to take advantage of available accommodations, students must register with Disability Resource Office (<https://dro.dasa.ncsu.edu/>) located at Holmes Hall, Suite 304, 2751 Cates Avenue, Campus Box 7509, 515-7653. For more information on NC State's policy on working with students with disabilities, please see the Academic Accommodations for Students with Disabilities Regulation at: <http://policies.ncsu.edu/regulation/reg-02-20-01>

Anti-Discrimination Statement: NC State University provides equality of opportunity in education and employment for all students and employees. Accordingly, NC State affirms its commitment to maintain a work environment for all employees and an academic environment for all students that is free from all forms of discrimination. Discrimination based on race, color, religion, creed, sex, national origin, age, disability, veteran status, or sexual orientation is a violation of state and federal law and/or NC State University policy and will not be tolerated. Harassment of any person (either in the form of quid pro quo or creation of a hostile environment) based on race, color, religion, creed, sex, national origin, age, disability, veteran status, or sexual orientation also is a violation of state and federal law and/or NC State University policy and will

not be tolerated. Retaliation against any person who complains about discrimination is also prohibited. NC State's policies and regulations covering discrimination, harassment, and retaliation may be accessed at <http://policies.ncsu.edu/category/campus-environment/non-discrimination> or <http://oied.ncsu.edu/>. Any person who feels that he or she has been the subject of prohibited discrimination, harassment, or retaliation should contact the Office for Institutional Equity & Diversity (OIED) at 515-3148.

Online Course Evaluations: Online class evaluations will be available for students to complete during the last two weeks of class. Students will receive an email message directing them to a website where they can login using their Unity ID. All evaluations are confidential; instructors will never know how any one student responded to any question, and students will never know the ratings for any instructor. Evaluation website: <http://go.ncsu.edu/cesurvey>
Student help desk: classeval@ncsu.edu
More information about ClassEval: <http://oirp.ncsu.edu/classeval/for-students/>

Health and Well-Being Resources: These are difficult times, and academic and personal stress is a natural result. Everyone is encouraged to take care of themselves and their peers. If you need additional support, there are many resources on campus to help you:

1. Counseling Center: <https://counseling.dasa.ncsu.edu/>
2. Health Center: <https://healthypack.dasa.ncsu.edu/>
3. If the personal behavior of a classmate concerns or worries you, either for the classmate's well-being or yours, we encourage you to report this behavior to the NC State CARES team: <https://advising.dasa.ncsu.edu/resources-for-advisors/advisors-toolkit/cares/>
4. If you or someone you know are experiencing food, housing or financial insecurity, please see the Pack Essentials Program: <https://dasa.ncsu.edu/pack-essentials/>

Other Important Resources:

1. Keep Learning, tips for students opting to take courses remotely: <https://dasa.ncsu.edu/students/keep-learning/>
2. Protect the Pack FAQs: <https://www.ncsu.edu/coronavirus/frequently-asked-questions/>
3. NC State Protect the Pack Resources for Students: <https://www.ncsu.edu/coronavirus/reactivating-campus/resources-for-students/>
4. Introduction to Zoom for students: <https://youtu.be/5LbPzzPbYEW>
5. Learning with Moodle, a student's guide to using Moodle: <https://moodle-projects.wolfware.ncsu.edu/course/view.php?id=226>