MatSE 598 DT: Density Functional Theory

Fall 2025

Schedule

TR 11:00–12:20pm in 119 English Building

Course content

- Reading:
  - Richard M. Martin's **Electronic Structure: Basic Theory and Practical Methods** 2nd ed. online
  - David S. Sholl and Janice A. Steckel's **Density Functional Theory: A Practical Introduction** online
- Assignment upload: my.matse.illinois.edu/courses/upload, select MSE 598
- Quantum Espresso website
- Course website: courses.grainger.illinois.edu/mse598dt; PDF syllabus

Instructor

Dallas R. Trinkle (dtrinkle@illinois.edu; 308 MSEB in the west stairwell).

- Professor in Materials Science and Engineering (joined Univ. Illinois in 2006)
- Computational materials science
  - Crystalline defects (dislocations, point defects, interfaces) from density functional theory
  - Development of new algorithms, computational tools
  - Solid solution softening / strengthening, pipe diffusion
  - Methods development: interatomic potentials, dislocation boundary conditions, DFT
  - General theory of diffusion

Scope

- Fundamental theory behind density-functional theory calculations
- Basics of electronic structure and correlation
- Practical aspects of DFT calculations
- Controlled and uncontrolled approximations in DFT
- Applications of DFT calculations to problems in materials science

Objectives

Students will be able to

(a) use quantum mechanics to derive the fundamental equations of Kohn-Sham DFT
(b) understand the practical choices in a modern DFT calculation
(c) perform DFT calculations with error estimates
(d) apply DFT to problems of scientific interest
(e) critically read the scientific literature on DFT

Prerequisites

- Electronic Properties of Materials/Condensed Matter Physics
  - MSE 304, PHYS 460/560, or equivalent.
- Introductory Quantum Mechanics
  - PHYS 486, or equivalent
- Thermodynamics
  - MSE 401/500, CHEM 484, PHYS 427, ME 404 or equivalent

Homework

Roughly every two weeks there will be homework assigned; a set of problems to be worked individually, and uploaded electronically.

Projects

In the next few weeks, we will form teams that balance interests, programming ability, and experience. The team will be given (i) a collective grade for a status report and its presentation in class, (ii) a collective grade for the final report, and (iii) a collective grade for the presentation of the final results. For your status report and final report we will use peer review, which will also be part of your grade.

We expect the project itself to take into account:

- *Scientific research.* Each project should be research oriented, something concerning DFT calculations and with a scientific component.
- *Algorithm development.* This could involve an optimization of an existing code or algorithm, a new implementation, some interesting science, the use of new computer architectures, or databases.
- *Presentation.* We expect a written report from each team that explains your project. This should include graphics, literature links, and potentially web references. With your permission, we may use these in future years as examples of class projects. You will also give an oral presentation of your project at the end of the semester during the time allotted for the final exam.

Prior to the status report, two slides used for this presentation need to be submitted. It needs to outline a problem (*Scientific research*) and explain what the team will do to solve it (*Algorithm development*), according to the criteria given above. Also the final reports and the final presentations

need to be submitted electronically. Late submissions will be penalized by 50 % for each day late. *If you have any questions about the suitability of your project please get in touch with the instructor.*

Minute paper

In the final minutes of Thursday's class, we will conclude with a **minute paper** which helps to synthesize your understanding of the week's lectures, think about your questions, and help me adjust content as needed. This will be done electronically using the link: illinois.edu/fb/sec/1088468787. There, you will have three questions:

1. What are the two (or more) most significant (central, useful, meaningful, surprising) things you have learned during this week?
2. What main question(s) remain for you?
3. Is there anything that you did not understand?

I will compile the questions, organize them, and may answer or address some of them at the beginning of the following week. Your responses also help me to adjust the course as needed.

Grading

- **40%** Homework
- **10%** Minute papers (drop lowest)
- **5%** Status report
- **15%** Final presentation
- **15%** Final report
- **5%** Peer review Status report
- **10%** Peer review Final report

Letter grades:

- A+ (>97), A (>93), A- (>90)
- B+ (>87), B (>83), B- (>80)
- C+ (>77), C (>73), C- (>70)
- D+ (>67), D (>63), D- (>60)

Expectations

To succeed in this class, you will need to

- study assigned reading material before coming to class, and formulate questions;
- participate in the class;
- make sure you understand the homework problems and solutions;
- propose, develop, implement, and present DFT calculations together with a team;
- seek out help when you have trouble.

Obtaining help: The main way to obtain help are through Slack, asking your peers or the instructor. In cases of emergencies related to assignments (e.g., illness) you should contact your professor at the earliest possible opportunity.

Formal and Informal Accommodations

I am committed to assisting students requiring special accommodations for circumstances that are registered with the DRES Student Services Department. These formal accommodations should be discussed with me as early as possible in the semester or as soon after DRES approval as possible.

If you are not formally registered with DRES and have anxiety, depression, learning disabilities, or other issues that affect your ability to fully participate and learn in this class, you are encouraged to check-in with me so we can determine together the kind of support you need to thrive in this class. Please set up a meeting with me via email.

Inclusion and Diversity

I value all students regardless of their background, race, religion (creed), ethnicity, gender, gender expression, age, country of origin, disability status, marital status, sexual orientation, or military status, etc., and am committed to providing a climate of excellence and inclusiveness within all aspects of the course. If there are aspects of your culture or identity that you would like to share with me as they relate to your success in this class, I am happy to meet to discuss. Likewise, if you have any concerns in this area of facing any special issues or challenges, you are encouraged to discuss the matter with me (set up a meeting via email) with an assurance of full confidentiality (only exception being mandatory reporting of academic integrity / code violation and sexual harassment). **Harassment or discrimination of any kind will not be tolerated.**

Anti-Racism and Inclusivity Statement

The intent is to raise student and instructor awareness of the ongoing threat of bias and racism and of the need to take personal responsibility in creating an inclusive learning environment.

The Grainger College of Engineering is committed to the creation of an anti-racist, inclusive community that welcomes diversity along a number of dimensions, including, but not limited to, race, ethnicity and national origins, gender and gender identity, sexuality, disability status, class, age, or religious beliefs. The College recognizes that we are learning together in the midst of the Black Lives Matter movement, that Black, Hispanic, and Indigenous voices and contributions have largely either been excluded from, or not recognized in, science and engineering, and that both overt racism and micro-aggressions threaten the well-being of our students and our university community.

Learning Environment

The effectiveness of this course is dependent upon each of us to create a safe and encouraging learning environment that allows for the open exchange of ideas while also ensuring equitable opportunities and respect for all of us. Everyone is expected to help establish and maintain an environment where students, staff, and faculty can contribute without fear of personal ridicule, or intolerant or offensive language. If you witness or experience racism, discrimination, micro-aggressions, or other offensive behavior, you are encouraged to bring this to the attention of the course director if you feel comfortable. You can also report these behaviors to the Office of the Vice Chancellor for Diversity, Equity and Inclusion (OVCDEI). Based on your report, OVCDEI members will follow up and reach out to students to make sure they have the support they need to

be healthy and safe. If the reported behavior also violates university policy, staff in the Office for Student Conflict Resolution may respond as well and will take appropriate action.

Religious Observances

Illinois law requires the University to reasonably accommodate its students' religious beliefs, observances, and practices in regard to admissions, class attendance, and the scheduling of examinations and work requirements. You should examine this syllabus at the beginning of the semester for potential conflicts between course deadlines and any of your religious observances. If a conflict exists, you should notify your instructor of the conflict and follow the procedure at ODOS to request appropriate accommodations. This should be done in the first two weeks of classes.

Sexual Misconduct Reporting Obligation

The University of Illinois is committed to combating sexual misconduct. Faculty and staff members are required to report any instances of sexual misconduct to the University's Title IX Office. In turn, an individual with the Title IX Office will provide information about rights and options, including accommodations, support services, the campus disciplinary process, and law enforcement options.

A list of the designated University employees who, as counselors, confidential advisors, and medical professionals, do not have this reporting responsibility and can maintain confidentiality, can be found here: wecare.illinois.edu confidentiality.

Other information about resources and reporting is available here: wecare.illinois.edu.

Family Educational Rights and Privacy Act (FERPA)

Any student who has suppressed their directory information pursuant to Family Educational Rights and Privacy Act (FERPA) should self-identify to the instructor to ensure protection of the privacy of their attendance in this course. See FERPA info for more information on FERPA.

Academic Integrity

You are bound by the University Honor Code in this course. Any violation of the Honor Code will result in disciplinary action.

Students are responsible for producing their own work. Collaborative interaction is encouraged, but each student must do their own individual prelecture work, and contribute their own work to the group. **Plagiarism will not be tolerated, and verified incidents will result in all parties receiving a zero and formal academic sanctions.** Students are responsible for familiarizing themselves with the definition of and penalties for plagiarism in Section I-401 of the UIUC Student Code. Note that plagiarism includes "copying another student's paper or working with another person when both submit similar papers without authorization to satisfy an individual assignment."

Changes to syllabus

May occur as deemed necessary by the professor; they will be announced and the updated syllabus posted on the course website.

Accessing files

The Univ. Illinois library has access to a huge variety of electronic resources; this plus additional online resources will be our references. Many can be accessed from the library's website, or via the campus VPN. Alternatively, you can take advantage of the library proxy. This is done by appending `proxy2.library.illinois.edu` to the web address; when reloaded, you will be asked for Univ. Illinois authentication, and then will be able to access the resource as if you were on campus. In general, this authentication is required only once per session. So, the website

`http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.113.025504`

would become

`http://journals.aps.org.proxy2.library.illinois.edu/prl/abstract/10.1103/Phy`

Alternatively, install the Proxy Bookmarklet which makes it extremely easy to use the proxy. I highly recommend this method.

Lecture topics and reading calendar

Tuesday	Thursday	*reading and assignments*	*topics*
8/26	8/28	**M** 1.–, **SS** 1.2 **RV** 2.– (minus 2.10, 2.15, 2.16)	Introduction, Schrodinger equation
9/2	9/3	**RV** 3.–, 4.3, 4.4, 4.6, 6.1–6.5 11.3, 12.2	Solutions to the SE, bra-ket notation
9/9	9/11	**M** 4.3	variational principle, symmetry, Bloch's theorem, spin, Pauli exclusion principle
9/16	9/18	**M** 3.1, 3.2, 3.6, 3.7	Many-body problems, Slater determinant, Hartree-Fock
9/23	9/25	**M** 3.3, 3.4, **RV** 13.2	Perturbation theory, forces, Born-Oppenheimer approximation
9/30	10/2	**M** 5.1, 5.2, 6.2	Free electron gas, Fermi statistics, Thomas-Fermi
10/7	10/9	**M** 6.3–6.7, 7.1–7.8	Hohenberg-Kohn and Kohn-Sham
10/14	10/16	**M** 4.1, 4.7, 12.3	Crystal structures, density of states, empty crystals, tight-binding
10/21	10/23	**M** 4.2, 4.6, 8.–, 12.1–12.3	Basis functions, Brillouin zone integration, exchange-correlation functionals
10/28	10/30	**M** 11.2–11.8, 11.11–11.12, 17.1–17.5	Pseudopotentials and PAW, full potential methods
11/4	11/6	**M** 12.7, 13.2	Real-space grids, self-consistency, iterative diagonalization
11/11	11/13	**SS** 3.5, 8.–	Total energy, geometry optimization, stress, band structure calculations

Tuesday	Thursday	*reading and assignments*	*topics*
11/18	11/20	**M** 13.5, **SS** 5.–, 6.3, 9.–	Supercells for defects, elastic constants and phonons, kinetics (NEB and MD), magnetism?
~~11/25~~	~~11/27~~	*no class*	*Thanksgiving break*
12/2	12/4	**M** 9.1–9.4, 9.6–9.7	Hybrid potentials, dispersion interactions, GGA+U
12/9	*12/12*	*Friday Dec. 12 final project presentations*	GW

Reading assignments correspond with chapters / sections in: **M** (Martin), **SS** (Sholl and Steckel), **RV** (Rajasekar and Velusamy), **IL** (Ibach and Lueth)

Background reading

You may want to review the following references to refresh yourself on particular prerequisite topics:

- S. Rajasekar and R. Velusamy, **Quantum Mechanics I**. doi:10.1201/9781003172178. There are multiple useful chapters here:
  - Chapter 2 covers the Schrodinger equation and wave fucntions
  - Chapter 3 covers operators, eigenvalues, and eigenfunctions
  - Chapter 4 covers many solvable systems
  - Chapter 6 covers matrices and bra-ket notation
  - Chapter 11 and 12 cover angular momentum and the H atom
- H. Ibach and H. Lueth, **Solid-State Physics**. (Springer Berlin Heidelberg: Berlin, Heidelberg, 2010). doi:10.1007/978-3-540-93804-0. There are multiple useful chapters here:
  - Chapters 2 and 3 cover lattices and crystals
  - Chapters 4 and 5 cover phonons
  - Chapters 6 and 7 cover electrons and band structure