PHYS 6800-001. **Selected Topics in Solid State Physics.**

**Instructor and office hours**

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Spring 2026 – TuTh 11:00-12:20 – Phys 116
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**Course Outline:** This course introduces advanced computational methods for electronic structure calculations, focusing on Density Functional Theory and related techniques. Students will explore quantum mechanics and solid-state physics fundamentals, then progress to topics such as Kohn-Sham equations, pseudopotentials, lattice dynamics, electron-phonon interactions, and optical properties. Advanced modules include non-equilibrium Green's functions, molecular dynamics, and the Car-Parrinello method. Hands-on laboratories and individual projects will reinforce theoretical concepts through practical applications using state-of-the-art software and high-performance computing environments.

**Instructional material and textbooks**

The instructional materials will be based on cutting edge, contemporary research, with an emphasis on problems in nano-scale physics and engineering. Lectures will draw upon several textbooks, among which:

- R. Lasar, *Computational Materials Science*, MRS Press
- R.M. Martin, *Electronic Structure*, Cambridge
- D.S. Sholl and J.A. Steckel. *Density Functional Theory, a practical introduction*. Wiley

**Supplementary Materials:** Electronic notebooks and other online materials will be provided by the instructor to complement the learning experience.

**Prerequisites:**

- Laboratory work and students' projects will use the *quantum*-ESPRESSO software package (http://www.quantum-espresso.org).
- Basic knowledge of the UNIX/LINUX programming environment.
- Basic knowledge of Python. For those unfamiliar with Python, LearningPython.org is a recommended starting point. Numerous free online resources are also available to cultivate sufficient Python knowledge essential for course success.
- A foundational understanding of quantum mechanics, solid state physics and linear algebra.

**Course Objectives:**

At the end of this course students should be able to identify the best computational strategy to solve the electronic structure problem at hand, apply the correct procedure

and interpret the results with a good knowledge of the known methodological limitations. Student should be able to run a state-of-the-art software package for electronic structure calculations, design specific computational *experiments* and be able to assess the precision and accuracy of the results. They should also be able to appreciate and comprehend seminars and scientific papers related to the subject of the course. Computer laboratories and students' projects will be designed to accomplish these goals

Student Participation: Students are encouraged to bring individual projects, which will be integrated as part of the class workload.

## Syllabus

- Overview of quantum mechanics concepts
- Overview of solid-state physics concepts
- The many-body problem and Density Functional Theory
- Kohn-Sham equations and bands in crystals:
    - Plane waves
    - Localized orbitals
    - Augmented functions
- Pseudopotentials in electronic structure theory
- Local Density Approximation and beyond
- Basic algorithms and functionalities
    - Forces and stresses
    - Density Functional Perturbation Theory
        - lattice dynamics
        - electron-phonon interactions and superconductivity
        - dielectric properties, Raman and IR scattering
    - Excitation spectra and optical properties
    - Scanning Tunneling Microscopy simulations
    - Non-collinear magnetism and spin-orbit interaction
    - Spontaneous polarization, localization and Berry's phases
    - Wannier functions
    - Non-equilibrium Green's functions and electronic transport in nanostructures
    - Chemical reactions and transition state searches: the Nudged Elastic Band method
- Statistical mechanics and Molecular Dynamics
    - Integrators, ergodicity, and statistical errors
    - Thermostats
    - Dynamic properties and correlation functions
- The Car-Parrinello method and other advanced simulation techniques

Laboratories will cover topical subjects such as graphical applications for visualization of the data, hands-on exercises, overview of programming environments for high-performance computing, etc.
Other subjects can be discussed upon completion of the required modules.

## Grading

Grading will be based on the successful completion of the modules in the allotted time. Students will return their assignments as jupyter notebooks through Canvas.

## Course Technology & Skills

*Minimum Technology Requirements*

- Computer

*Computer Skills & Digital Literacy*

- Using Canvas
- Downloading and installing software
- Knowledge of programming in Python
- Knowledge of the Linux environment

## Attendance

Students are expected to attend class meetings regularly and to abide by the attendance policy established for the course. It is important that you communicate with the professor and the instructional team prior to being absent, so you, the professor, and the instructional team can discuss and mitigate the impact of the absence on your attainment of course learning goals. Please inform the professor and instructional team if you are unable to attend class meetings because you are ill, in mindfulness of the health and safety of everyone in our community.

## UNT POLICIES

### Academic Integrity Policy

Academic Integrity Standards and Consequences. According to UNT Policy 06.003, Student Academic Integrity, academic dishonesty occurs when students engage in behaviors including, but not limited to cheating, fabrication, facilitating academic dishonesty, forgery, plagiarism, and sabotage. A finding of academic dishonesty may result in a range of academic penalties or sanctions ranging from admonition to expulsion from the University. [Insert specific sanction or academic penalty for specific academic integrity violation.

In this course, you are encouraged to use Generative AI (GenAI) tools for code development (Claude, GPT-5, etc. and to develop skills for a GenAI-oriented workforce. This use will help us stay technically proficient and ethically grounded. However, GenAI should complement, not replace, your critical thinking or our course materials. If something seems unclear, please seek clarification.
In line with the UNT Honor Code, all work you submit must be your own. Using GenAI tools without attribution or relying on them to complete assignments violates academic integrity and will be addressed according to university policy.

### ADA Policy

UNT makes reasonable academic accommodation for students with disabilities. Students seeking accommodation must first register with the Office of Disability Accommodation

(ODA) to verify their eligibility. If a disability is verified, the ODA will provide a student with an accommodation letter to be delivered to faculty to begin a private discussion regarding one's specific course needs. Students may request accommodations at any time, however, ODA notices of accommodation should be provided as early as possible in the semester to avoid any delay in implementation. Note that students must obtain a new letter of accommodation for every semester and must meet with each faculty member prior to implementation in each class. For additional information see the ODA website at disability.unt.edu.

### Emergency Notification & Procedures

UNT uses a system called Eagle Alert to quickly notify students with critical information in the event of an emergency (i.e., severe weather, campus closing, and health and public safety emergencies like chemical spills, fires, or violence). In the event of a university closure, please refer to Blackboard for contingency plans for covering course materials.

### Retention of Student Records

Student records pertaining to this course are maintained in a secure location by the instructor of record. All records such as exams, answer sheets (with keys), and written papers submitted during the duration of the course are kept for at least one calendar year after course completion. Course work completed via the Blackboard online system, including grading information and comments, is also stored in a safe electronic environment for one year. Students have the right to view their individual record; however, information about student's records will not be divulged to other individuals without proper written consent. Students are encouraged to review the Public Information Policy and the Family Educational Rights and Privacy Act (FERPA) laws and the University's policy. See UNT Policy 10.10, Records Management and Retention for additional information.

### Acceptable Student Behavior

Student behavior that interferes with an instructor's ability to conduct a class or other students' opportunity to learn is unacceptable and disruptive and will not be tolerated in any instructional forum at UNT. Students engaging in unacceptable behavior will be directed to leave the classroom and the instructor may refer the student to the Dean of Students to consider whether the student's conduct violated the Code of Student Conduct. The University's expectations for student conduct apply to all instructional forums, including University and electronic classroom, labs, discussion groups, field trips, etc. The Code of Student Conduct can be found at deanofstudents.unt.edu/conduct.

### Access to Information - Eagle Connect

Students' access point for business and academic services at UNT is located at: my.unt.edu. All official communication from the University will be delivered to a student's Eagle Connect account. For more information, please visit the website that explains Eagle Connect and how to forward e-mail: eagleconnect.unt.edu/

### Student Evaluation Administration Dates

Student feedback is important and an essential part of participation in this course. The student evaluation of instruction is a requirement for all organized classes at UNT. The survey will be made available during weeks 13, 14 and 15 of the long semesters to provide students with an opportunity to evaluate how this course is taught. Students will receive an email from "UNT SPOT Course Evaluations via IASystem Notification" (no-

reply@iasystem.org) with the survey link. Students should look for the email in their UNT email inbox. Simply click on the link and complete the survey. Once students complete the survey they will receive a confirmation email that the survey has been submitted. For additional information, please visit the SPOT website at http://spot.unt.edu/ or email spot@unt.edu.

Sexual Assault Prevention

UNT is committed to providing a safe learning environment free of all forms of sexual misconduct, including sexual harassment sexual assault, domestic violence, dating violence, and stalking. Federal laws (Title IX and the Violence Against Women Act) and UNT policies prohibit discrimination on the basis of sex, and therefore prohibit sexual misconduct. If you or someone you know is experiencing sexual harassment, relationship violence, stalking, and/or sexual assault, there are campus resources available to provide support and assistance. UNT's Survivor Advocates can assist a student who has been impacted by violence by filing protective orders, completing crime victim's compensation applications, contacting professors for absences related to an assault, working with housing to facilitate a room change where appropriate, and connecting students to other resources available both on and off campus. The Survivor Advocates can be reached at SurvivorAdvocate@unt.edu or by calling the Dean of Students Office at 940-565- 2648. Additionally, alleged sexual misconduct can be non-confidentially reported to the Title IX Coordinator at oeo@unt.edu or at (940) 565 2759.