

MSEN 5377, Spring 2025

Computational Physics of Nanomaterials

Course Syllabus

Course Information

<i>Course Number/Section</i>	MSEN 5377-001
<i>Course Title</i>	Computational Physics of Nanomaterials
<i>Credits</i>	3
<i>Term</i>	Spring 2025
<i>Days and Times</i>	Tu & Th 2:30-3:45 pm
<i>Location</i>	ECSN 2.316

Professor Contact Information

<i>Professor</i>	Massimo Fischetti
<i>Office Phone</i>	972-883-5724
<i>Email Address</i>	max.fischetti@utdallas.edu
<i>Office Location</i>	NSERL 3.708
<i>Office Hours</i>	By appointment

Course Pre-requisites, Co-requisites, and/or Other Restrictions

MSEN 6319 or equivalent course on Quantum Mechanics

Course Description

Review of Quantum Mechanics and crystal structure. The role of nanostructures in Materials Science. Introduction to numerical methods (integration, finite differences) and programming. Theory and computational techniques I: Atomic and electronic structure of nanostructures. Theory and computational techniques II: Electronic transport.

Student Learning Objectives/Outcomes

Provide a basic understanding of:

- The importance of nanostructures in the present technology
- Numerical techniques
- Theoretical and computational methods to deal with the atomic and electronic structure of systems at the nanometer scale
- Theoretical and computational methods to deal with electronic and ionic transport in these systems
- Theoretical and computational methods to deal with electronic and ionic transport in these systems

Suggested Reading Material

The Lecture Notes (together with homework assignments and additional material) will be posted on the class Web page, https://personal.utdallas.edu/~mvf100020/MSEN5377_S25.html. No single textbook will be used. Possible additional sources may be:

- T. Young and M. J. Mohlekamp, "Introduction to Numerical Methods and MATLAB Programming for Engineers", (Ohio University Press, Athens, OH, 2010): A general introduction to numerical methods and programming with MATLAB examples
- K. Ohno, E. Esfarjani, and Y. Kawazoe, "Computational Materials Science", (Springer-Verlag, Berlin, Heidelberg, 1999): Excellent compendium of computational methods to deal with the atomic and electric structure of materials.
- R. W. Hockney and J. W. Eastwood, "Computer Simulations Using Particles", (Institute of Physics, Bristol, UK, 1988): "The" text about numerical methods employing particles

Homework assignments and additional material will be posted on the class website:

https://personal.utdallas.edu/~mvf100020/MSEN5377_S25.html

Grading Policy

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|--------------|-----|---|
| • Homework | 40% | (4-to-6 homework assignments due approximately every 2 weeks) |
| • Project I | 30% | (due around late-March/early-April) |
| • Project II | 30% | (due by the end of classes) |

Course & Instructor Policies

<i>Make-up exams</i>	Only under extreme circumstances at the Professor's discretion
<i>Extra credit</i>	Not available
<i>Late work</i>	Accepted only for serious and well-documented reasons. Only partial credit will be given.
<i>Class attendance</i>	<i>Although not required</i> , attendance is STRONGLY encouraged since some topics will be presented and discussed only in class. In addition, see "Class Participation" below.

Class Participation

Regular class participation is expected. Students who fail to participate in class regularly are inviting scholastic difficulty. A portion of the grade for this course is directly tied to your participation in this class. It also includes engaging in groups or other activities during class that solicit your feedback on homework assignments, readings, or materials covered in the lectures (and/or labs). Successful participation is defined as consistently adhering to University requirements, as presented in this syllabus. Failure to comply with these University requirements is a violation of the [Student Code of Conduct](#).

Class Recording

Students are expected to follow appropriate University policies and maintain the security of passwords used to access recorded lectures. Unless the AccessAbility Resource Center has approved the student to record the instruction, students are expressly prohibited from recording any part of this course. Recordings may not be published, reproduced, or shared with those not in the class, or uploaded to other online environments except to implement an approved AccessAbility Resource Center accommodation. Failure to comply with these University requirements is a violation of the [Student Code of Conduct](#).

Comet Creed

This creed was voted on by the UT Dallas student body in 2014. It is a standard that Comets choose to live by and encourage others to do the same:

"As a Comet, I pledge honesty, integrity, and service in all that I do."

Accommodation for Students with Disabilities

Please review [the section](#) within the UT Dallas Syllabus Policies and Procedures webpage.

Academic Support Resources

Please visit the [Academic Support Resources](#) page to view the University's academic support resources for all students.

UT Dallas Syllabus Policies and Procedures

Please visit the [Syllabus Policies](#) page to view the University's policies and procedures segment of the course syllabus. Please review the catalog sections regarding the [credit/no credit](#) or [pass/fail](#) grading option and withdrawal from class.

The descriptions and timelines contained in this syllabus are subject to change at the discretion of the Professor.

