Special Topics Course

Carbon and Molecular Nanoelectronics

Objective

In this course we will use carbon nanotubes to understand quantum transport as the foundation for all emerging nanoelectronic devices.

Overview

Carbon nanotubes, which were discovered only 15 years ago, are considered potential candidates for a diverse set of electronic applications such as transistors, interconnects, sensors, nanoelectromechanical (NEMS) switches, optoelectronic devices, and electron guns. The topics covered in this course are therefore vital for students interested in various applications of carbon nanotubes in many different fields.

In this course, carbon nanotubes and graphene nanoribbons will be used as a framework to understand electron transport in nano-scale structures in general. In virtually all nano-scale devices, whether they are silicon nanowires, ZnO nanowires and nanobelts, graphene nanoribbons, or carbon nanotubes, electrons are confined in one or two dimensions. Electron transport in low-dimensional devices is distinctly different from its classical form leading to unprecedented behaviors. We will explore novel electronic phenomena in low-dimensional systems and the limitations and opportunities that they pose to future devices and circuits.

We will also learn how to use first-principles calculations to obtain the electronic properties of carbon nanotubes. These techniques can be used to extract the electronic properties of other emerging nano-scale devices such as graphene nanoribbons. Finally, practical applications of carbon nanotubes and graphene such as transistors, interconnects and sensors will be discussed.

Prerequisites

General understanding of electrical circuits, electronic devices, and linear algebra is required. No prior acquaintance with quantum mechanics is required. All necessary QM concepts will be covered in the course. Familiarity with MATLAB is needed for homework assignments.

Textbook

Quantum Transport: From Atoms to Transistors, Supriyo Datta, Cambridge University Press, 2005 (available at GIT Bookstore).

Recommended Books

Quantum Mechanics for Scientists and Engineers, David A. B. Miller, Cambridge University Press, 2008.

Helpful resources on this book such as solutions to selected problems, animations, and viewgraphs are available at:
http://www-ee.stanford.edu/~dabm/QMbook.html

Electronic Transport in Mesoscopic Systems, Supriyo Datta, Cambridge Studies in Semiconductor Physics and Microelectronic Engineering (No. 3), Cambridge University Press, 2005.

The few sections from the above two books that will be used in the class will be distributed during the course. The two books are also on reserve in library.

Grade:

The final grade will be calculated as follows:

Homework	40%
Term paper	20%
Exam 1, Feb. 19	20%
Exam 2, April 16	20%

Homework assignments are an important component of this course. They are designed to make you master the material presented in class, prepare you for upcoming classes, and in some cases, complement what is taught in the class. A major part of assignments will be done with MATLAB. Your textbook has many MATLAB codes which can help you with writing such codes. You may discuss homework assignments with your classmates and also use the codes in your textbook as a guide. However, what you turn in must be your own work.

By Week 11, you are expected to have chosen a specific application of carbon nanotubes, graphene nanoribbons, or another nanomaterial to write a term paper on it. Original ideas for new applications of these materials or new operation mechanisms are strongly encouraged and will result in bonus credit. The goal of this project is to use the course material and your creativity to propose and/or model novel nanoelectronic devices, not writing term papers that are pure literature surveys.

Outline:

Weeks 1 & 2: Course Overview and Introduction to Quantum Mechanics
Week 3 & 4: Free Electrons in Low Dimensional Systems
Week 5: Finite Difference Method and Self Consistent Solutions
Week 6: Basic Functions and Density Matrix
Week 7 & 8: Bandstructure Calculations, Graphene bandstructure
Week 9: Carbon Nanotubes and Graphene Nanoribbons
Week 10: Effective Mass Hamiltonian
Week 11: Self Consistent Solutions to Schrodinger's and Poisson's Equations
Week 12: Coherent Transport Modeling
Week 13: Non-coherent Transport
Weeks 14–15: Potential Applications of Carbon Nanomaterials

Office Hours:

M-W 2-3 p.m.

Molecular and Carbon Nanoelectronics

1. Overview, From Microelectronics to Nanoelectronics

Introduction to Schrödinger equation

2. Simple Rationalization of Schrödinger’s (time-independent) equation
3. Simple Examples: Electrons in a Box
4. Simple Rationalization of the Time-Dependent Schrödinger Equation
5. Concept of Group Velocity

Electron Transport in Low Dimensional Systems (Free Electrons)

6. Electrons in One Dimension, Fermi Distribution, Quantum Resistance, Number of Conduction channels (Exercise: 3D wires, density of states)
7. Electron Scattering, Electron Mean Free Path, Ohm’s Law,
8. Coherent Transport, Optical Analogies, Voltage Probes
9. Quantum capacitance and Kinetic Inductance

Electron Transport in Crystals

10. Method of Finite Difference
    a. Matrix representation of Schrodinger Equation
    b. Eigenvalues and Eigenvectors
    c. Examples (particle in a box and the difference between analytical and matrix solutions)
11. Method of Finite Difference (Continued)
    a. Boundary conditions
    b. Particles in a 3D box
    c. Spherical Coordinates
12. Self consistent.
13. Basic functions (Math)
14. Basic functions (Conceptual significance)
15. Density Matrix
16. Bandstructure (1D)
17. 1Bandstructure (Generalization, e.g. 2D)
18. Subbands (Nanotubes, zone folding)
19. Subbands (Graphene Nanoribbons)
20. Density of States
21. graphene nanoribbons
22. Effective Mass Hamiltonian
23. Density Matrix and Quantum Capacitance

Devices

24. Level broadening and Local density of states
25. Self Energy
26. Life Time
27. Coherent Transport
28. Transmission
29. NEGF Numerical Solutions
30. Phonon Emission

31. Non-coherent Transport

Carbon Nanotube and Graphene Applications

32. Interconnects
33. Transistors
34. Sensors
35. Other applications