COURSE: ECE730 Topic 29

COURSE TITLE: **Computational Nanoelectronics**

INSTRUCTOR: Prof. Youngki Yoon
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LECTURE HOURS: TBD

DESCRIPTION:

The purpose of this course is to convey a new viewpoint to understand the current flow in nanoscale devices. Great success of nanotechnology has brought numerous opportunities in nanoelectronics, but the properties of nanosystems cannot be well described by a classical way where empirical fitting parameters have been widely adopted. This course provides the conceptual framework to explore nanoscale materials and devices based on quantum mechanics. Through hands-on coding assignments, students can grasp physical insights into confined systems and carrier transport in novel semiconductor devices.

EXPECTED BACKGROUND: Basic matrix algebra

COURSE/TEACHING OBJECTIVES:

This course will help students with no or limited background in computational nanoelectronics

- ≅ acquire the basic concepts of quantum mechanics within the relevant topics of nanoscale devices,
- ≅ obtain in-depth understanding of nanomaterials and nanoscale devices,
- ≅ acquire the knowledge and skill in the field of atomistic quantum simulation, and
- ≅ develop hands-on coding experience for electronic band structure and device simulation.

SYLLABUS:

01. ***Introduction*** (1 week)
Energy level diagram; Electron/Hole conduction; Origin of current flow; Quantum of conductance

02. ***Schrödinger equation*** (1 week)
Hydrogen atom; Finite difference method; Boundary conditions

03. ***Self-consistent electrostatics*** (1 week)
Self-consistent field; Multi-electron picture

04. ***Basis functions*** (1 week)
Basis functions as a computational tool; Basis functions as a conceptual tool; Equilibrium density matrix

05. ***Band structure of semiconductors*** (1 week)
Chain of atoms; Brillouin zone; Reciprocal lattice; Band structure of common semiconductors

06. ***Subbands of nanomaterials*** (1 week)
Quantum wells, wires and dots; Graphene and carbon nanotubes; Density of states; Minimum resistance of a wire

07. ***Nanoscale MOS Capacitance*** (1.5 weeks)
Model Hamiltonian; Electron density; Quantum capacitance

08. ***Open systems*** (1.5 weeks)
Contacts; Level broadening; Local density of states

09. ***Carrier transport*** (2 weeks)
Non-equilibrium density matrix; Transmission; Coherent/Incoherent transport

10. ***Project Presentation*** (1 week)

CODING ASSIGNMENT:

Assignment will be given for the topics covered in the class. Matlab (or equivalent software package) will be used. (No prior programming experience is required.) Examples are as follows:

- ≅ Current through a simple system with constant density of states
- ≅ Charge in a nanosystem with self-consistent field
- ≅ Eigenvalues under different boundary conditions
- ≅ Band structure of confined systems such as carbon nanotubes and graphene
- ≅ Transmission of a nanoscale device

TEXTBOOK:

There is no required textbook.

GENERAL REFERENCES:

- ≅ Quantum Transport: Atom to Transistor, Supriyo Datta, Cambridge University Press (2013).
- ≅ Lessons from Nanoelectronics: A New Perspective on Transport, Supriyo Datta, World Scientific Publishing Company (2012).

MARKING SCHEME:

- ≅ Assignment: 30%
- ≅ Term Project: 20%
- ≅ Final Exam: 50%