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:**

**MARKING SCHEME:**
- Assignment: 30%
- Term Project: 20%
- Final Exam: 50%