Pontificia Universidad JAVERIANA Cali

[VIGILADA MINEDUCACIÓN Res. 12220 de 2016]

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EL DECANO DE LA FACULTAD DE INGENIERÍA Y CIENCIAS
INFORMA QUE:

En el periodo 2020-2 (julio-noviembre) se dictaron los cursos que se relacionan a continuación, para los estudiantes del Doctorado de Ingeniería y Ciencias Aplicadas de la Pontificia Universidad Javeriana Cali, en el marco del Programa Ómicas:

Asignatura	Profesores
Biología Computacional	Carolina Clavijo Buriticá y Andrés Jaramillo
Química Orgánica	Drochss Valencia
Ciencia de los Materiales	Adriana Gómez
Seminario de ética y filosofía de la ciencia	Diego Agudelo
Computación Científica	Luis Tobón
Aprendizaje Automático	Diego Linares
Nanoelectrónica	Andrés Jaramillo
Bases Formales de Computación	Carlos Ramírez

Cordialmente,

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ENGINEERING DOCTORATE
Faculty of Engineering

Nanoelectronics
400IGE005

Pre-requisites: Physical Chemistry

Motivation

Modern technology is characterized by its emphasis on miniaturization. Perhaps the most striking example is electronics, where remarkable technological progress has come from reductions in the size of transistors, thereby increasing the number of transistors possible per chip.

With more transistors per chip, designers are able to create more sophisticated integrated circuits. Over the last 35 years, engineers have increased the complexity of integrated circuits by more than five orders of magnitude. This remarkable achievement has transformed society. Even that most mechanical creature of modern technology, the automobile, now typically contains half its value in electronics

Gordon Moore, a co-founder of Intel, noted the industry's history of steady increases in complexity. The eponymous Moore's law states the complexity of an integrated circuit, with respect to minimum component cost, will double in about 18 months. Over time the "law" has held up pretty well.

But exponential trends cannot continue forever.

Already, in CPUs there are glimmers of the fundamental barriers that are approaching at smaller length scales. It has become increasingly difficult to dissipate the heat generated by a CPU running at high speed. The more transistors we pack into a chip, the greater the power density that we must dissipate. For example, the power density of modern CPUs is higher than 150 W/cm2. For perspective, note that the power density at the surface of the sun is approximately 6,000 W/cm2. The sun radiates this power by heating itself to 6000 K. But we must maintain our CPUs at approximately room temperature. The heat load of CPUs has pushed fan forced convection coolers to the limits of practicality. Beyond air-cooling is water-cooling, which at greater expense may be capable of removing several hundred Watts from a 1cm2 sized chip. Beyond water-cooling, thermoelectric conversion might be a solution.

But as electronic devices approach the molecular scale, our traditional understanding of electronic devices will also need revision. Classical models for device behavior must be abandoned. Many electrons in modern transistors electrons travel "ballistically" – they do not collide with any component of the silicon channel. Such ballistic devices cannot be analyzed using conventional transistor models. To prepare for the next generation of electronic devices, this class teaches the theory of current, voltage and resistance from atoms up.

In this course we discuss "The Quantum Particle", by introducing the means to describe electrons in nanodevices. In early transistors, electrons can be treated purely as point particles. But in nanoelectronics the position, energy and momentum of an electron must be described probabilistically. We will also need to consider the wave-like properties of electrons, and we will include phase information in descriptions of the electron, and discuss how this forms the basis for two, three and more terminal devices.

Course description

The 16 week course will introduce the basic concepts behind the development of modern nanoelectronic systems and devices required to understand their design, optimization and operational limits.

Goals and Objectives

The course is meant as a foundational introduction to the field of nanoelectronics that exposes students to the first-principles theory of quantum level transport. It is aimed at experimentalists and theorists in chemistry, materials science, chemical engineering, applied physics, biochemistry, physics, geophysics, and from other engineering programs with an interest in characterizing, optimizing or designing materials and understanding material properties and phenomena.

After successful course completion, the attendant will:

- Achieve a conceptual and theoretical understanding of electronic structure methods from nanoelectronics
- Acquire the practical knowledge and skills about first-principles quantum chemistry methods, to compute electronic band structures, transmission spectra, conductance, and IV curves.
- Learn how to use quantum chemistry codes to characterize electronic/optical properties in materials.

Prerequisites

- Basic knowledge of C/C++, Python and Unix is required. Will also be used during the course lectures as well as in class assignments. Mathematica or Matlab are a plus.
- Background required in differential equations, statistical and classical mechanics, and linear algebra.
- The students must have successfully completed a course on Physical Chemistry.

Course contents and calendar

1) *Introduction (2 sessions)*
    a) *Electron Wavepacket Propagation*
    b) *The hydrogen atom*
    c) *The Born-Oppenheimer approximation*
    d) *Hybrid Orbitals*
2) *The Electronic Structure of Materials (2 sessions)*

3) *The Quantum Particle (2 sessions)*
4) *The Quantum Particle in a Box (2 sessions)*
5) *Two Terminal Quantum Dot Devices (2 sessions)*
6) *Two Terminal Quantum Wire Devices (2 sessions)*
7) *Field Effect Transistors (2 sessions)*
8) *Fundamental Limits in Computation (2 sessions)*

Simulation packages and tools

We will be using different modeling and simulation tools to demonstrate and apply the theory and methods described during the lectures, among these:

- *SeQuest general purpose electronic structure code for periodic systems, slabs or finite molecules (Sandia National Laboratory, SNL, http://dft.sandia.gov/Quest/)*
- *Quantum Espresso general purpose electronic structure code for periodic systems, slabs or finite molecules (http://www.quantum-espresso.org)*
- *GAMESS general ab initio quantum chemistry package (http://www.msg.chem.iastate.edu/gamess/)*
- *Jaguar (commercial package http://www.schrodinger.com/Jaguar/)*

A brief tutorial on the use of a QM package will be offered. The student will be responsible for learning other tools that he/she chooses to use for the same level of calculations as those listed here.

Other useful tools:

- VMD visual molecular dynamics (http://www.ks.uiuc.edu/Research/vmd/)
- Ovito molecular visualizer (http://www.ovito.org)
- Avogadro molecule builder (http://avogadro.cc/wiki/Main_Page)

How to study for this course

Attend lectures, read the class notes ahead of time (if applicable), read the suggested scientific literature recommended during class sessions, practice simulation runs on local cluster, and solve all the assignments, including the class project individually (unless explicitly stated otherwise). Teamwork is encouraged, but you must hand in your own results for all assignments.

Homework will be handed out each week during the first 8 weeks, and it will use generally available computer software implementing the basic methods on applications aimed at exposing the students to understanding how to use atomistic simulations to solve problems. Each calculation requires making decisions on the specific approaches and parameters relevant and how to analyze the results. The lowest homework score will be dropped from the final grade.

No late assignments will be accepted.

The midterm will require each student to submit a proposal for a project using the methods of this course to solve a research problem that can be completed in the final 8 weeks. The homework for the last 8 weeks is to turn in a one-page report on progress with the project.

The final is a research report describing the calculations and conclusions.

Evaluation

Homework assignments	30%
Midterm	20%
Final	20%
Project	30%

References

1. Introduction to Nanoelectronics: Marc Baldo, MIT OpenCourseWare, Publication May 2011.