Lectures on First-Principles Simulations of Materials: Fundaments and Applications to Nano-electronics, Thermal Transport and Electrochemistry

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Abstract:
The course will provide a general introduction to first principles modeling of materials, going from a overview of the field to more specialized and current topics of research. The presentation of the fundaments will be focused on the topics of Molecular Dynamics simulations, and of Density Functional Theory. Then, applications of these techniques to several topics of current interest wil be discussed, addressing both the theoretical tools developed to describe specific physical processes and to compute the relevant properties, and showing their use in the context of experimental results. These topics will include electronic transport in nanoscale devices (for nanoelectronics and molecular electronics), thermal transport of materials, and the interface between electrolytes and electrified electrodes (relevant for electrochemistry applications such as batteries). Other topics and applications can be discussed according to the interests of the students.

Lectures Program (tentative): five Lectures of 2h each.

Lecture 1: Fundaments of Computer Simulations in Materials: Overall View.
- Sampling the configuration space: Monte Carlo and Molecular Dynamics
- Solving the quantum mechanical problem: approximations
- Density Functional Theory and beyond

Lecture 2: Electronic Transport in Nanoscale Devices
- Landauer Formulation
- Non-Equillibrium Green's Functions and Density Functional Theory
- Applications to molecular electronics and nanoscale devices

Lecture 3: Thermal transport in Materials: Thermal conductivity
- Approaches to compute Thermal Conductivity from First Principles
- Application to bulk crystals and disordered materials and liquids
- Applications in nanostructures

Lecture 4: Simulations of the electrochemical interface
- Complexity of the interface between electrolytes and electrodes
- Approaches to address electrochemical processes from first principles
- Application cases

Lecture 5: Open topics (to be discussed with the students)

Tentative calendar:

Week 1	Monday June 17, 10 to 12 am, room L1.4	Wednesday June 19, 10 to 12 am, room L1.4
Week 2	Monday June 24, 10 to 12 am, room L1.6	Thursday June 27, 10 to 12 am, room L1.6
Week 3	Thursday July 4, 10 to 12 am, room L1.6	

In addition to the above lectures, Professor Ordejón will give a Department/Cnr Seminar on Tuesday, June 11 at 4 pm. Title: “DFT and QM/MM simulations of the electrochemical interface”. More details will follow.

Pablo Ordejón - Brief CV

Pablo Ordejón obtained his PhD (1992) from the Autonomous University of Madrid. He has been Postdoctoral Researcher at the University of Illinois (USA), Assistant Professor at the University of Oviedo, and Permanent Researcher at the ICMAB-CSIC in Barcelona. In 2007 he moved to the Catalan Institute of Nanoscience and Nanotechnology (ICN2), of which he has been director since 2012. He has published more than 220 scientific articles, with more than 35,000 citations.

His research interest focuses on the simulation of the properties of materials at the atomic level, using methods based on quantum mechanics. He is known for developing efficient numerical methods for very large scale simulations, with a reduced scaling with the size (number of atoms) of the systems being studied. He is one of the main co-developers of SIESTA, an open source DFT code for the study of complex materials, used by hundreds of groups worldwide.

Ordejón has been head of the Condensed Matter Physics area of the Spanish Agency of Scientific Evaluation (ANEP) and of the Physics and Engineering Panel of the Spanish Supercomputing Network, and coordinator of the Physics area of the Gadea Foundation. He is a Fellow of the American Physical Society and a member of the Academia Europaea, and received the Narcis Monturiol medal from the Government of Catalonia. He is currently a Trustee of the Barcelona Institute of Science and Technology (BIST). He was co-founder of SIMUNE Atomistics SL, a spin-off company that provides materials simulation services to industrial clients.