Student profile

This tutorial is open to graduate students, postdocs, young scientists and engineers who are interested in learning about state-of-the-art computational methods for materials science.

Registration fees

Student: 900 Dhs;
Researcher: 1600 Dhs;
Industrial: 3500 Dhs
The fees cover all the lectures, restauration and accommodation for the full tutorial period.

Certificate

A training certificate will be delivered to the attendees attesting their performance in Modeling the Electronic Structure of Materials during the tutorial directly after the end of the tutorial.

For registration, contact MSN

TEL: +212-626-906-135
Tel: +212-651-632-456
E-mail: msn@um6p.ma

MOHAMMED VI
POLYTECHNIC UNIVERSITY

Quality of the Tutorial

- Excellence in teaching
- Interdisciplinary approach
- Courses in English/French

Ideal student campus and facilities

The students can enjoy outstanding facilities such as:
Learning Center, Conference Hall, Residence, Cantine, Cafeteria...

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TUTORIAL IN COMPUTATIONAL
MATERIAL SCIENCE
KINETIC MONTE CARLO (KMC)
20-22 JUNE 2019

MOHAMMED VI
POLYTECHNIC
UNIVERSITY

UM6P at the heart of Africa

PROGRAM

The Mohammed VI Polytechnic University, UM6P, is an institution oriented toward applied research and innovation. UM6P puts research and innovation at the service of development of the African continent, and is thus committed to economic and human development. UM6P's positioning allows it to consolidate Morocco's forward-looking position in research innovation and entrepreneurship, through the implementation of a unique partnership approach and the strengthening of its education and training offer. Thanks to the efforts of all its components, the University is fast becoming relevant to Morocco's and Africa's future.

MSN, MATERIALS SOLUTIONS FOR A SUSTAINABLE FUTURE

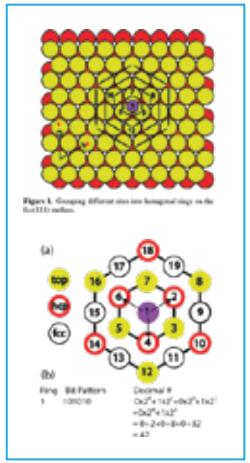
The Materials Science and Nano-engineering (MSN) is part of Mohammed VI Polytechnic University (UM6P) research center departments. MSN's vision is based on interdisciplinary research. The competence of its researchers and the relevance of its research topics are adapted to meet different national and global issues.

MSN develops high-level fundamental and applied research in materials science and nano-engineering. As its research areas are related to materials science, MSN has adopted a research strategy and a clear vision, based on the following axes

4 PARCOURS

- ENERGY MATERIALS
- COMPOSITES & POLYMERS
- PHOSPHATE & BY-PRODUCTS
- SURFACE TECHNOLOGIES

Modeling of materials requires simulations and tools at different time and length scales. When information is sought at the electronic level, quantum mechanics based tools are needed. These tools are relatively expensive as they require the electrons to be treated explicitly. These tools, in general, treats systems at the nano-meter and pico-second length and time scales, respectively. When it is necessary to study a system at much larger time and length scales, and details of the electronic structure can be treated implicitly, molecular dynamics simulations can be used to study the evolution of a system in time and space at scales near the micro-second and micro-meter. In these simulations, the vibrational dynamics of the system are treated explicitly, including the anharmonic effects. However, when the importance is focused on the evolution of the system at time scales of the order of minutes, hours or even days (scales of crystal growth for example).



It is not possible to use molecular dynamics simulations. In these cases, the vibrational dynamics are not treated explicitly (but implicitly in "pre-factors) and activation barriers become the central piece of information into the simulations. These simulations are called Kinetic Monte Carlo (KMC). Using transition state theory (TST), one allows the system to evolve from an equilibrium configuration to another equilibrium configuration through a probabilistic game built on the energy costs for the system to transition from a configuration to another, for all possible transitions. When a system has long-range order and when the evolution in time and space of the system at hand occurs via a small number of processes, one uses a pre-defined "catalog" of processes to perform KMC simulations.

Lecturers

Professor Abdelkader Kara
University of Central Florida, USA

DAY 1

Afternoon: Welcome Reception and Registration

DAY 2

Morning: Introduction to multi-scale simulations of Materials
Afternoon: Introduction to Kinetic Monte Carlo

DAY 3

Morning: Applications of Kinetic Monte Carlo
Afternoon: Certificate Reception.