CECAM

Centre Européen de Calcul Atomique et Moléculaire

SISSA

i|o|m
Istituto Officina dei Materiali

CECAM Summer School on Atomistic Simulation Techniques for Material Science, Nanotechnology and Biophysics
Trieste, 14 - 30 June 2017

SISSA and CNR-IOM are jointly organizing the CECAM Summer School on Atomistic Simulation Techniques for Material Science, Nanotechnology and Biophysics in Trieste, on 14 - 30 June 2017.

The purpose of the School will be threefold: (i) providing students with a basic but detailed overview of the theoretical foundations and numerical methods of quantum mechanical (QM) simulations of molecular and extended systems; (ii) training them to solve quantum mechanical problems in practice, either implementing simple numerical codes from scratch or using existing QM codes for selected applications; (iii) giving an overview of the domains of current interesting research problems in material and biochemical science.
At the end of the school the students should have a clear idea of the importance of quantum mechanical molecular simulations; they should be aware of the problems that are still open and are at the center of current research efforts and should have the capability of developing their own simple code for performing a simulation or an analysis.

This is the 8th edition of this summer school, which every year has received more than 100 applications, with about 25 of them being accepted.

In 2017 the School will be entirely focused on quantum mechanics and in particular will be devoted to electronic properties of materials, chemical- and bio-molecules. The duration of the School is two weeks (plus the pre-school). Morning lectures are followed by afternoon hands-on tutorials in the computer lab.

For those interested, a three-day introduction to scientific programming and Linux environment (pre-school) with hands-on tutorial sessions on some simple physics problems will be offered on 14-16 June 2017.

Program of the School

WEEK 1: Electronic Structure (Introduction to band theory, LCAO method, plane waves and pseudopotentials, density functional theory, self-consistent calculations, forces and stress, density functional perturbation theory, introduction to Quantum ESPRESSO).

WEEK 2: Quantum Chemistry (Introduction to electronic and molecular structure, mathematical methods for electronic structure theory in chemistry, Hartree Fock and Post-Hartree Fock methods, conformational search and finite temperature simulations, QM/MM).

Registration Fee

A registration fee (200 Euro) will be required to the accepted candidates and reimbursed to students who will have fully attended the school. The organizers will cover accommodation (14 nights), lunches and dinners at SISSA (Monday to Friday), public transportation and social dinner. Lodging expenses will be covered also during the pre-school. Limited support toward travel expenses can be provided in exceptional cases, based on fund availability.

How to apply

To apply please visit the following website:

http://democritos.sissa.it/school2017

ORGANIZERS

Stefano de Gironcoli
(SISSA, Trieste)

Andrea Dal Corso
(SISSA, Trieste)

Alessandra Magistrato
(CNR-IOM, Trieste)

LECTURERS

Michele Cascella (Oslo University)
Andrea Dal Corso (SISSA)
Stefano de Gironcoli (SISSA)
Alessandra Magistrato (CNR-IOM)
Angelo Rosa (SISSA)
Mauro Stener (Trieste University)

**DEADLINE
for requesting participation
31st March 2017**