Predictive Modelling and Computational Methods for Organic Electronics

Date: 10 June 2014

Venue: San Geminiano,University Conference Center, Modena (Italy)

Chairpersons: Elisa Molinari (Uni Modena & Reggio Emilia, and CNR-Istituto Nanoscienze, Modena) and Claudio Zannoni (UNIBO, Bologna, Italy)

Lecturers:

Fabrizia Negri (UNIBO, Dip. Chimica Ciamician)

KarstenHannewald (Humboldt-Universität, Berlin)

Andrea Ferretti (CNR-IstitutoNanoscienze, Modena)

Otello Roscioni (UNIBO, Dip. Chimica Industriale "Toso Montanari")

Luca Muccioli (UNIBO, Dip. Chimica Industriale "Toso Montanari")

Casalegno (POLIMI)

Meeting Overview

The one-day course aims at presenting modeling and computational approaches to organic electronics materials, nanostructures, devices.The course is a forum for graduate students, post-docs, and young scientists already acquainted with standard electronic structure calculations or with knowledge on their features, and wishing to enter orprogress into advanced computational methods for the calculation of electronic properties and transport in organic electronics. The School aims at stimulating the interest for potential and perspectives of thesetechniques from model structures to realistic systems.

Thelectures will have a tutorial character andwill overview principles, latest progress and challenges, including charge transport both coherent and via hopping in various organic materials in the bulk and at their interfaces.

Program

Morning session*(Chair Zannoni/Molinari)*

- 9:00 – 10:00 am: Fabrizia Negri (UNIBO, Dip. Chimica Ciamician): “Structure-property relationships in organic semiconductors”
- 10:00 – 11:00 am: KarstenHannewald (Humboldt-Universität, Berlin):"Polaron Transport in Organic Molecular Crystals: Theory and Ab-Initio Modelling"
- 11:00 – 11:30 am: Coffee Break (with Poster session)

- 11:30 – 12:30 am: Andrea Ferretti (CNR-IstitutoNanoscienze, Modena): “Coherent electron transport through single molecules: insights from ab-initio calculations”
- Lunch: 12:30 am –2:00 pm

Afternoon session*(Chair Zannoni/Molinari)*

- 2:00–3:00 pm: Otello Roscioni (UNIBO, Dip. Chimica Industriale "Toso Montanari"): “Molecular dynamics simulations of organic thin films on inorganic supports.”
- 3:00–4:00 pm:Luca Muccioli (UNIBO, Dip. Chimica Industriale "Toso Montanari"): "Modelling organic/organic interfaces: structure and energy levels"
- 4:00 – 4:30 pm: Coffee Break (with Poster session)
- 4:30-5:30 pm: Mose' Casalegno (POLIMI): “Dynamical modeling methods in organic electronics: the simulation of device behavior at the nanoscale”.
- 5:30-6:00 pm: Wrap-up discussion
- 6:00 - 7:30 pm, Poster session, with beverages and snacks

Application Instructions

The meeting will feature 6one-hour lectures by scientists experts of Modeling and Computational Methods, one poster session and a round table with Q/A. A proactive participation by attendees is encouraged through 15-minute discussion for each lecture. All applicants must include an abstract of the poster.

Registration

Registration is done on the ICOE 2014 web site, although is independent of the ICOE 2014 conference. Registration fee is 75 € before deadline, and 100 € after deadline or at the conference site, and includes lunch, coffee breaks, and aperitif. A certificate of attendance will be released.
