

Industrial Forum for Multiscale Materials Modelling and Training

11-13 September 2013

Bologna, Italy.

Programme

Wednesday 11th September

8.30-9.00	Registration
9.00-9.30	Welcome and address by MMM@HPC project coordinator, W. Wenzel (KIT)
9.30-10.00	Our hope in the Multi-Scale Simulation for Electronics Devices, Yuichi Tokita (Sony).
10.00-10.30	Molecular insights into charge transport in conjugated materials for applications in organic electronics, Yoann Olivier (Uni. Mons)
10.30-11.00	Organic Semi-conductors for Advanced Electronics: Detailed Atomistic Simulation of the Structural, Packing and Morphological properties of Amorphous and Crystalline Poly-Alkyl-Thiophene (PAT) systems, Orestis Alexadis (Uni. Patras)
11.00-11.30	Coffee break
11.30-12.00	Predictive simulations of Liquid Crystals: from Displays to Organic Electronics, Claudio Zannoni (Univ. of Bologna)
12.00-12.30	Functionalization of graphitic materials and control: an ab-initio study, Veilimir Meded (KIT)
12.30-14.00	Buffet Lunch
14.00-14.30	Li-Ion battery ageing: challenges of the multi-scale modeling, Mathias Gerard (CEA-LITEN)
14.30-15.00	Overview of HPC Services for Modelling at Cineca, Claudio Arlandini (Cineca).
15.00-15.30	TBD, Luigi Occhipinti (ST Microelectronics)
15.30-16.00	Coffee break
16.00-16.30	Multi-Scale molecular dynamics in soft matter, Valentina Tozzini (CNR, NEST-Pisa)
16.30-17.00	

Thursday 12th September

8.30-9.00	Registration
9.00-9.30	Computational Screening Strategies of OLED Materials for Mass Production Process, Hyeonho Choi (Samsung)
9.30-10.00	Multiscale Modelling Approaches: Understanding and Designing Organic Semiconductors, Christian Lennartz (BASF).
10.00-10.30	The Quantum ESPRESSO project and foundation, Stefano Baroni (SISSA)
10.30-11.00	Large scale parallel materials simulations with LAMMPS, Axel Kohlmeyer (ICTP)
11.00-11.30	Coffee
11.30-12.00	Multiscale modelling of organic devices by Kinetic Monte Carlo, Alison

	Walker (Univ. of Bath)
12.00-12.30	"Industrial Applications of Multi-Scale Modeling on Organic Materials - A paradigm shift for the invention and optimization of organic materials", Simon Widmaier (Nanomatch)
12.30-14.00	Buffet Lunch
14.00-14.30	Some applications of mathematical and numerical methods for material modelling, Paolo Ferrandi (MOXOFF, Milan)
14.30-15.00	Modeling composite materials using TRUE multiscale technology and HPC infrastructure, Dario Mendolicchio (Altair)
15.00-15.30	Materials modelling with HPC: current practice, trends and the challenges of petascale, Andrew Emerson (Cineca).
15.30-16.00	Coffee break
16.00-16.30	TBC
16.30-17.00	Workshop Close

Friday 13th September – Training Session

8.30-9.00	Registration	
9.00-9.30	Introduction and Demonstration	
9.30-12.30	Hands-on training session	
12.30-14.00	Buffet Lunch	
14.00-16.00	Training	Project Meeting (MMM@HPC partners only)
16.00-17.30		