Simulation Methods for Condensed Matter Systems
GCI - Computational Physics Group

CNISM Meeting

13-06-2012

Physics Department of 'La Sapienza' University

Members

- Prof. G. Ciccotti
- Dr. Sara Bonella
- Prof. Carlo Pierleoni
- Dr. Michele Monteferrante
- Dr. Letizia Chiodo
- Dr. Adolfo Poma
- Dr. Antonio Deiana
- Dr. Elisa Liberatore
- Marco Micciarelli

Our Realm

developing and application of computational methods, at various length scales, for condensed phase materials: static, dynamical, electronic and optical properties

systems: surface/interfaces, biomolecules, polymers, liquid, amorphous and crystalline phases

Methods
- Classical MD, quantum MD
- Coarse Grained
- Classical and Quantum MonteCarlo
- DFT and Many Body derived methods

Main Research Lines

- Rare events methods for energy and biology (Ciccotti-Bonella)
- Mixed quantum-classical dynamics methods (Ciccotti-Bonella)
- Coupled electron-ion Quantum MonteCarlo Pierleoni)
- Classical MD applied to Nanostructures (Bonella, Chiodo)
- Excited states dynamics (Bonella)
- Electronic and optical properties of nanostructures and molecules (Chiodo)

solid state physics

- ab initio study of reduced-dimensionality systems (surfaces, interfaces, nanocrystals) and of organic-inorganic hybrid systems

- Ground state properties: Density Functional Theory DFT

- Excited state properties:Time Dependent DFT, and Many Body Perturbation Theory based techniques (GW, sc-COSHEX, BSE)

Most Recent Applications

- hydropathicity of small biologic molecules
- hydrogen and hydrogen-helium in extreme conditions (J. Chem. Phys. 134, 184505 (2011))
- polymeric solutions (Soft Matter 8, 5151-5167 (2012))
- silver self-aggregated nanostructures (Nanoscale, 4, 2362-2371 (2012))
- solid state hydrogen storage in sodium alanates (Phys. Chem. Chem. Phys. 13, 10546 (2011))
- oxides for PV and PC applications (J. Chem. Phys. **135**, 244704 (2011))
- d-metal surfaces (Phys. Rev. Lett. **108**, 126402 (2012))

please refer to http://abaddon.phys.uniroma1.it/index.php for the complete list of publications