Due to a problem with our former web server, the list of the seminars held between May 2007 and July 2009 is currently unavailable. We're working to recover the data, and hope to update this page soon!

May 15, 4:00 pm, Aula 5 Edificio Fermi, Department of Physics

Prof. Keith E. Gubbins - Center for High Performance Simulation (CHiPS) and Department of Chemical and Biomolecular Engineering North Carolina State University, Raleigh

Confinement effects on chemical reactions - toward an integrated rational catalyst design
Chemical reactions are often carried out in nano-structured materials, which can enhance reactions due to interactions with the reacting mixture, high surface area and confinement effects. We present a systematic study of reactions in confinement, using ab initio and semi-classical methods. We first consider the influence of steric hindrance on the equilibrium and kinetics for the rotational isomerizations of small hydrocarbons, and show that confinement can lead to reaction rates that vary doubly exponentially with pore width. We further consider several reactions to produce hydrogen, including the decomposition of formaldehyde[1] , methane and water[2] on carbon surfaces, with and without the presence of defects and added transition metal atoms. These results provide examples of the influence on reaction mechanism, yield and rate of electrostatic interactions with the supporting material, surface defects and surface curvature.

[1] Erik E. Santiso, Aaron M. George, Keith E. Gubbins, Marco Buongiorno-Nardelli, J. Chem. Phys., 125, 084711 (2006).
[2] M.K. Kostov, E.E. Santiso, A.M. George, K.E. Gubbins, M.B. Nardelli, Phys. Rev. Lett. 95 (2005) 136105.

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April 30, 3:00 pm, Aula Conversi Edificio Marconi, Department of Physics

Dott. Federica Lo Verso - Institut für Theoretische Physik II, Heinrich-Heine-Universtität, Düsseldorf

Telechelic star-like micelles: conformation and phase behaviour
Telechelic micelles, i.e. micelles constituted by polymers carrying functionalized endgroups, are a versatile and readily tunable system, giving rise to a rich variety of macroscopic phase behavior. In this class, polymer aggregates that carry attractive end-groups are relevant to determine the principles behind the intra and/or inter-molecular association, to understand biomembranes, proteins and for synthesis of novel materials.

We investigated the conformational and structural properties of functionalized star-shaped polymeric aggregates [1], by Molecular Dynamic simulations and analytical theory, and we established the functionality- and polymerization-number dependence of the transition temperature from open to collapsed macroparticle structure [2].

Moreover, we modified the strength of the effective arm-arm attraction, i.e. the ratio between the number of repulsive and attractive monomers per arm, and we studied the interplay between micellization and fluid-fluid phase transition by employing monomer-resolved Monte Carlo simulations on a lattice [3].

The characterization of the morphologies of the dense phases (micelles, lamellae, networks) will be briefly discussed.

[1] D. Vlassopoulos ,T. Pakula, G. Fytas, M. Ptsikalis and N. Hadjichristidis J. Chem. Phys. 111,

1760 (1999).
[2] F. Lo Verso, C. N. Likos, C. Mayer, and H. Löwen Physical Review Letters 96, 187802 (2006).
[3] S.K. Kumar and A.Z. Panagiotopoulos Physical Review Letters 82 5060 (1999).

April 27, 3:00 pm, Aula Conversi Edificio Marconi, Department of Physics

Prof. Daniel Borgis - Université d'Evry, Département de Physique et Modélisation Laboratoire de Modélisation des Systèmes Moléculaires Complexes, Evry

Density Functional Theory of Solvation

We describe a density functional theory approach to solvation in molecular solvents. The solvation free-energy of a complex solute can be obtained by direct minimization of a density functional, instead of the thermodynamic integration scheme necessary when using atomistic simulations. In the homogeneous reference fluid approximation, the expression of the free-energy functional relies on the knowledge of the direct correlation function of the pure solvent. After discussing general molecular solvents, we present a generic density functional describing a dipolar solvent and we show how it can be reduced to the conventional implicit solvent models when the solvent microscopic structure is neglected. With respect to those models, the functional includes additional effects such as the microscopic structure of the solvent, the dipolar saturation effect, and the non-local character of the dielectric constant. We show how this functional can be minimized numerically on a three-dimensional grid around a solute of complex shape to provide, in a single shot, both the average solvent structure and the absolute solvation free energy. We also show how to extend the approach to a multicentre model of acetonitrile, using an angular grid representation of the density and of the direct correlation functions.

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March 14, 5:00 pm, Aula Conversi Edificio Marconi, Department of Physics

Prof Eckhard Spohr - Institut für Energieforschung, Forschungszentrum, Jülich

A Microscopic View of the Polymer Electrolyte Membrane Fuel Cell. Atomistic Simulations of Proton Generation and Transport
Polymer electrolyte membrane fuel cells are described. In direct methanol cells protons originate from dissociation of methanol on precious metal catalysts in aqueous media. The solvent role in stabilizing intermediates and enhancing proton desorption is studied by combined classical molecular dynamics (MD) - ab initio simulations. The interplay of molecular structure and proton mobility in individual membrane pores and membrane networks is also studied by MD.

February 19, 3:00 pm, Aula Conversi Edificio Marconi, Department of Physics

Prof Roland Winkler - Institut für Festkörperforschung Forschungszentrum Jülich

Mesoscale simulations of star polymers
A set of multiple-particle-collision (MPC) simulations to describe the dynamical behavior of complex fluids will be presented. The dependence of the physical properties of simple fluids, flexible molecules in solution, and colloids on the model parameters and the influence of the hydrodynamics interaction in the different situations will be analyzed with particular reference to star polymers.

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February 12, 3:00 pm, Aula 6 Edificio Fermi, Department of Physics

Prof Alessandro Laio - International School of Advanced Studies, Trieste, Italy

Folding of small proteins in explicit solvent by the combined use of metadynamics and replica exchange
We recently developed a method[1] that combines replica exchange[2] with metadynamics[3] and allows, with a moderate computational effort, the simultaneous reconstruction of the free energy as a function of a large number of variables. This allows simulating very complex reactions, like protein folding, in which the reaction coordinate is totally unknown. We will discuss applications of the methodology to the folding in explicit solvent of the TRP cage miniprotein and of the advillin headpiece C-terminal domain (cHP) and its Pro62Ala mutant. Our calculations allow, for these small proteins, the ab initio prediction of the folded state. For the advillin headpiece we find that the Pro62Ala mutation does not change the overall stability of the native state but it significantly alters the entropic contribution to the folding free energy. Therefore, the mutant is still folded at room temperature but is characterized by a lower unfolding temperature. This prediction was subsequently validated by NMR and CD

experiments.

1 Piana S. and Laio, submitted (2006).

2 Y. Sugita and Y. Okamoto, Chem. Phys. Lett. 314, 141 (1999).

3 Laio A. and Parrinello M., Proc Natl. Acad. Sci. USA, 99,12562 (2002).

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January 22 , 3:00 pm , Aula Touschek, Department of Physics

Prof Michel Mareschal - Universite' Libre de Bruxelles

Hydrodynamics at the nanoscale
Using Molecular Dynamics simulations, it has been observed that continuum descriptions remain valid up to atomic scales, whether in equilibrium or in non-equilibrium states. A somewhat impressive example is that of fluid hydrodynamic instabilities, when flow patterns emerge and fit the boundary conditions. The case of two-dimensional Bénard convection rolls will be discussed in more details in this presentation.

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Prof David Coker - Boston University

January 15 , 10:00 am, Aula Touschek, Department of Physics

Sampling quantum thermal initial conditions

January 16 , 10:00 am, Aula Touschek, Department of Physics

Vibrational relaxation and dephasing in electronic excited states for condensed phase systems

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