7th Workshop on Molecular Theories and Simulations
Gaeta (Latina), Hotel Summit, 16-18 May 2008

Organizing committee:
A. Amadei (Roma, TOV)
M. Aschi (L'Aquila)
A. Di Nola (Roma, La Sapienza)

Friday 16
18:00-18:35  Ambra Tarquini. Università di Roma ‘La Sapienza’
Theoretical and computational characterization of dilute ionic solutions under the effect of external electric field.

18:35-19:10  Stephan Lutz. University of Basel
Ligand migration in heme-proteins.

Saturday 17
9:30-10:05  Markus Meuwly. University of Basel
The role of higher CO-multipole moments in understanding the dynamics of photodissociated carbon monoxide in Myoglobin.

10:05-10:40  Marco D’Abramo. IRB Barcelona
Protein dynamics in electrospray conditions.

10:40-11:20  Coffee Break

11:20-11:55  Isabella Daidone. IWR Uni-Heidelberg
Hydrogen-bond driven loop closure kinetics in unfolded polypeptide chains.

11:55-12:30  Paolo Foggi. LENS Firenze
Time-resolved spectroscopy: what we learn about structure and dynamics of complex molecules.

13:00  Lunch

15:30-16:05  Modesto Orozco. IRB Barcelona
Simulation in nucleic acids, going to the genomic scale.

16:05-16:40  Antonella Fontana. Università di Chieti
Study of the aggregation behaviour of a series of block co-polymers in water.
16:40-17:20  Coffee Break

17:20-17:55  Massimiliano Anselmi. Università di Roma ‘La Sapienza’
The kinetics of ligand migration in crystalized Myoglobin as revealed by MD simulations.

17:55-18:30  Alessandro Grottesi. CASPUR Roma
Essential dynamics of the mitochondrial ADP/ATP carrier: dynamical role of odd-numbered helices.

18:30-19:05  Guoyng Qi. University of Norwich
Role of interdomain bending regions in ligand induced domain closure.

Sunday 18

9:00-9:35  Costantino Zazza. CASPUR Roma e Università di L’Aquila
An Electrochemical Controllable Nanospring.

9:35-10:10  Stephen Hayward. University of Norwich
New results on well-known biomolecular complexes using DynDom3D.

10:10-10:45  Riccardo Spezia. Universite' d'Evry Val d'Essonne
Modelling Collision Induced Dissociations by Direct Dynamics Simulations.

10:45-11:15  Coffee Break

Calculation of a Protein dielectric response using Molecular Dynamics simulations

11:50-12:25  Laura Zanetti. Università di Roma ‘La Sapienza’
Structural and Thermodynamic Characterization of a Beta-Hairpin Peptide in Solution: a MD Study of a Synthetic Analogue of Gramicidin S

12:25-13:00  Massimiliano Aschi. Università di L’Aquila
On the UV spectrum of water in condensed phase: a different interplay between experimentalists and theoreticians?

13:30   Lunch

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