4th Workshop on Molecular Theories and Simulations

Gaeta, 13-15 May 2005

Organizing committee:

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

Program

Friday 13

afternoon: welcome and rooming in.

Saturday 14

10:00-10:30	Alessandro Marrone (Universita' di Chieti) ***"DFT studies on trans and cis platin"***
10:30-11:00	Riccardo Spezia (Paris) ***"Theoretical study of neutral dipolar atom in water: structure, spectroscopy and formation of an excitonic state"***
11:00-11:30	Coffee break
11:30-12:00	Catherine Snow (University of Norwich) ***"Investigating the domain movements in Adenylate Kinase using essential dynamics sampling."***
12:00-12:30	Isabella Daidone (Universita' di Roma I) ***"Theoretical modelling of peptide folding kinetics"***
13:00	Lunch
15:30-16:00	Marco D'Abramo (Universita' di Roma I) ***"Further developments of PMM: new***

spectroscopic applications"

16:00-16:30 Alessandro Grottesi (University of Oxford)
"How do potassium channels gate? Insight from two study cases: Kirbac and Shaker"

16:30-17:00 Coffee break

17:00-17:30 Martin Ulmschneider (Universita' di Roma I)
"Implicit solvation forces for membrane protein simulations"

17:30-18:00 Tsjerk A. Wassenaar (University of Groningen)
"The purple membrane"

Sunday 15

9:30-10:00 Steven Hayward (University of Norwich)
"Comprehensive and non-redundant database of protein domain movements"

10:00-10:30 Dagmar Floeck (Universita' di Roma I)
"Protein misfolding and peptide aggregation studied by MD simulations"

10:30-11:00 Coffee break

11:00-11:30 Leonardo Guidoni (Universita' di Roma I)
"Mixed Quantum-classical MD simulations"

11:30-12:00 Andrea Amadei (Universita' di Roma II)
"Statistical mechanical modelling of chemical reactions"

12:00.12:30 Massimiliano Aschi (Universita' di L'Aquila)
Concluding discussion

13:00 Lunch

Hotel Summit - Gaeta (LT)
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