International School of Liquid Crystals
5th Course

Modeling of Complex Systems: From Single Molecules to Anisotropic Fluids and Beyond

Directors of the Course: A. Raudino, C. Zannoni
***E. Majorana* Centre for Scientific Culture, Erice**
22-26 October 2001

October 22

Afternoon: Arrival
21.15: Welcome Reception at the Marsala Lecture Hall (S. Rocco)

October 23

8.45-9.00	A. Raudino C. Zannoni	Welcome
9.0 - 10.00	**B. Roos**	From Atoms to Proteins - Quantum Chemistry in the 21st Century.

1st Session**: Chemical Kinetics**

10.00 –11.00	**V. Aquilanti**	Molecular Orientation in Gaseous Expansions and Scattering Measurements of Anisotropic Forces.
11.00 – 11.20		**Coffee Break**
11.20 - 11.50	G. Villani	Electron transfer: general aspects and open questions.
11.50 – 12.50	**G. Moro**	Stochastic analysis of bimolecular kinetics.
12.50 – 13.20	L. Ambrosone	The local potential and stability conditions in diffusing layers.

Lunch Break

2nd Session: **Computer Simulations of Chemical and Photochemical Processes**

16.00 – 17.00	**V. Schettino**	Molecular dynamics simulation of chemical reactions.
17.00 –17.30	C. Pomelli	A Theoretical study on π complexes between Bromine and sterically hindered olefins.
17.30 –18.30	**M. Persico**	Simulation of excited state dynamics in the presence of condensed phase.
18.30 – 19.00	C. Petrongolo	Electronic nonadiabatic dynamics in triatomic systems .

October 24

3rd Session**: Solvent Effects: Methods of Calculation and Applications**

8.30 – 9.30	**J. Tomasi**	Continuum and mixed continuum-discrete models to describe molecular properties in solution.
9.30 – 10.00	G. Graziano	Hydration of aromatic hydrocarbons.
10.00 – 10.30	S. Corni	Surface Enhanced Raman Scattering from a single molecule adsorbed on a metal particle aggregate: a theoretical study.
10.30-11.00	A. Tani	Simulazione di sistemi orientati con potenziali ottenuti da calcoli ab initio.
11.00 – 11.20		**Coffee Break**
11.20 – 13.20	**Poster Session**	

Lunch Break

4th Session: **Ordered Fluids**

16.00 – 17.00	**C. Zannoni**	Modelling and computer simulation of liquid crystals.
17.00 –17.30	G. Celebre	Anisotropic intermolecular potential of biaxial particles in nematics: comparison between Monte Carlo predictions and experiments.
17.30 –18.00	A. Ferrarini	A Continuum Model for the Molecular Structure Dependence of Electrostatic Interactions and Dielectric Properties in Liquid Crystals.
18.00 – 18.30	R. Berardi	A Monte Carlo study of the chiral columnar organizations of chiral discotic molecules.

October 25

5th Session: **Condensed Phase Models for Biological Systems**

8.30 – 9.30	**O.G. Mouritsen**	
9.30 –10.30	**P**. **DeBenedetti**	Theoretical approaches to quantitative relationships between chemical structure and biological activity.
10.30 –10.50		**Coffee Break**
10.50 – 11.50	**G. Orlandi**	The hole transfer in DNA: an ab initio calculation of the electronic coupling
11.50 – 12.20	A. Villa	Estimation of the relative protein-inhibitor binding free energies using molecular dynamics simulations.
12.20 – 12.50	M. Compiani	Stochastic models and neural networks to compute the folding times of all-α proteins
12.50 – 13.20	R. Improta	Role of long range and environmental effects in determining the conformational behavior of polypeptides.

Lunch Break

6th Session: **Complex Systems and Advanced Materials**

15.30 – 16.30	**G. Allegra**	Filled rubber: a mesoscopic bead-and-spring model of hard spherical particles in a polymer rubbery matrix.
16.30 – 17.00	G.B. Suffritti	Molecular Dynamics simulations of water confined in zeolites.
17.00 –17.30	E. Dalla	Investigation of residual nonaqueous phase liquid dissolution in porous media using pore-scale simulation.
17.30 – 18.00	M.A. Floriano	Micellization and Phase Separation in Model Diblock and Triblock Surfactants.
18.00 – 18.30	R. Noto	Molecular Dynamics study of the association of charged and uncharged pectin in aqueous solution.
18.30 – 19.00	G. La Manna	Studio della struttura di sistemi tubulari con unità peptidiche.
20.30	**Social Dinner**	

October 26 : Departure (n.b. only for those not staying for the second meeting)