

# COMPUTATIONAL MODELS FOR LIQUID CRYSTALS AND COMPLEX SYSTEMS

A CECAM Workshop

Erice (TP) July 13-18, 2002

Directors: Mike Allen, Paolo Pasini, Claudio Zannoni

**July 13**

**Afternoon: Arrival**

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

**July 14**

Dirac Lecture Hall (S. Domenico)

8.45 – 9.00

M. Allen  
P. Pasini  
C. Zannoni

**Welcome**

**Colloids and Polymers I**

9.00 – 10.00

G.J. Vroege

*Liquid-crystal phase transitions in suspensions of plate-like particles*

10.00 – 11.00

P.L. Taylor

*Simulation studies of solvent diffusion and the glass transition in polymers*

11.00 – 11.30

**Coffee Break**

11.30 – 12.30

B. Duenweg

*Hydrodynamic Screening in Semidilute Polymer Solutions: A Computer Simulation Study*

**Lunch Break**

**Liquid Crystals I**

16.00 – 17.00

L. Rull

*Computer simulation of liquid crystal interface.*

17.00 – 18.00

S. Zumer

*Simulations and modelling of defect dynamics in nematics*

18.00 – 19.00

*Phase diagram of discotic liquid crystals in bulk and in*

J. P. Ryckaert     *confined geometry*

## July 15

Dirac Lecture Hall (S. Domenico)

### Liquid Crystals II

8.30 – 9.30	C. Zannoni	<i>Computer simulations of real and virtual liquid crystals</i>
9.30 – 10.30	D.J. Photinos	<i>Molecular Simulations of the Liquid Crystalline Phases of Fan-Shaped Molecules</i>
10.30 – 11.00		<b>Coffee Break</b>
11.00 – 12.00	M. Glaser	<i>Atomistic simulation of smectics</i>
12.00 – 13.00	M. Wilson	<i>Simulation of LC polymers and dendrimers</i>

## Lunch Break

### Contributed papers and Poster Session

16.00 – 19.00

## July 16

Dirac Lecture Hall (S. Domenico)

### Colloids and Polymer II

8.30 – 9.30	G.J. Vroege	<i>Liquid-Crystalline Phase Behavior of a Colloidal Rod-Plate Mixture</i>
9.30 – 10.30	C. Caccamo	<i>Liquid-vapor and liquid-solid coexistence in a DLVO potential modelization of globular protein solutions</i>
10.30 – 11.00		<b>Coffee Break</b>
11.00 – 12.00	A. Louis	<i>Coarse graining polymers as soft colloids</i>
12.00 – 13.00	H. Loewen	<i>From basic interactions to phase diagrams: solutions of rod-like biomolecules</i>

## Lunch Break

### Half-day excursion

July 17

Dirac Lecture Hall (S. Domenico)  
**Liquid Crystals III**

8.30 – 9.30	S. Hess	<i>Phase behavior and structure of model liquid crystals and of fluids of Janus particles</i>
9.30 – 10.30	M. P. Allen	<i>Simulation and theory of inhomogeneous liquid crystals</i>
10.30 – 11.00		<b>Coffee Break</b>
11.00 – 12.00	G. Jackson	<i>The theory and simulation of polar and chiral phases.</i>
12.00 – 13.00	R. Berardi	<i>A Monte Carlo study of the chiral columnar organisations of chiral discotic mesogens</i>

**Lunch Break**

**Colloids and Polymers III**

15.00 – 16.00	M. Mueller	<i>Wetting of polymer solutions: Monte Carlo Simulations and Self-Consistent Field theory</i>
16.00 – 17.00	M. Ferrario	
17.00 – 17.15		<b>Coffee Break</b>
17.15 – 18.15	F. Schmid	<i>Liquid Crystals at surfaces</i>
20.30 – 24.00		

**SOCIAL DINNER**