

Nanostructured materials and membrane modelling and simulation

FORTH/ICE-HT, Patras, June 18-27, 2008

June 18, Wednesday			
Registration		09:00 - 11:30	
<i>A. Introductory Session - Modelling in Nanomaterials</i>			
Welcome - Course Description		11:30 - 13:00	Burganos V (FORTH)
Lunch			
Generic methods:			
Introduction to statistical mechanics and molecular simulation concepts		14:30 - 16:00	Theodorou D (NTUA)
Molecular Simulations - Monte Carlo		16:15 - 17:00	Mavrantzas V (FORTH)
June 19, Thursday			
Molecular Simulations: MD, kMC & TST		09:00 - 10:00	Vlachos D (Delaware)
Applying nonequilibrium thermodynamics principle to NEMD simulations		10:15 - 11:45	Edwards B (Tennessee)
Introduction to ab-initio methods and relation to nanomaterials research		12:00 - 13:15	Froudakis G (UCrete)
Lunch			
FP7, bilateral, national programmes		14:30 - 15:15	Hatzopoulou E. (IRC)
Lab tour		15:15 - 17:00	
June 20, Friday			
Coarse Graining in Molecular Simulations		09:00 - 10:15	Briels W (Twente)
Numerical solution of flow and diffusion equations		10:30 - 12:00	Tsamopoulos J (Upatras)
Simulation opportunities in nanocomposites research		12:30 - 13:30	Gerard JF (CNRS)
Lunch			
Poster session I		15:00 - 18:00	
Visit Patras Science Park		15:00 - 18:00	
June 21, Saturday			
Visit industrial zone			
June 22, Sunday			
Research ideas and proposals, interactions		10:00 - 13:00	
Poster session II		15:00 - 18:00	
June 23, Monday			
<i>B. Modeling of Material Structure</i>			
Atomic scale simulation of polymer structures		09:00 - 10:15	Hofmann D (GKSS)
Atomic scale simulation of nanomaterials: inorganic, hybrid, dense		10:30 - 12:00	Tocci E (Calabria)
Pore/grain models and 3D reconstruction		12:15 - 13:15	Kikkinides E (UWM)
Lunch			
Sintering: microscopic and geometric modelling		15:00 - 15:45	Pan J (Leicester)
Simulation methods to predict mechanical properties of nanomaterials		16:00 - 17:15	Rutledge G (MIT)
June 24, Tuesday			
<i>C. Modelling of Transport and Sorption</i>			
Phenomenological models of transport and sorption in porous materials		09:00 - 09:45	Bernauer B (ICTP)
Hierarchical modelling: concept and application to biofilm growth		10:00 - 11:00	Payatakes A (FORTH)
MC and MD in sorption and diffusion in polymers		11:30 - 12:15	van der Vegt N (MaxPlanck)
MC/MD in biopolymers		12:30 - 13:15	van der Vegt N (MaxPlanck)
Lunch			
Transport in carbon nanotubes		15:00 - 16:00	Quirke N (Imperial)
DFT modeling in XRD-assisted zeolite reconstructions		16:15 - 17:15	Berthomieu D (CNRS)

June 25, Wednesday			
	The Lattice Boltzmann method with applications to transport phenomena in porous materials	09:00 - 11:00	Krafczyk M (Germany)
	<i>D. Use of models to interpret experimental data</i>		
	Pore structure determination using mercury porosimetry	11:30 - 12:15	Tsakiroglou C (FORTH)
	Pore structure determination using adsorption / desorption: experiment and modelling	12:30 - 13:30	Seaton N (Edinburgh)
Lunch			
	Hg, N2 experiments	15:00- 17:00	Tsakiroglou C, Ioannides T (FORTH)
	Poster session III	15:00- 17:00	
June 26, Thursday			
	<i>E. Demonstration</i>		
	Demonstration of the use of an academic software: atomistic models of zeolites	09:00 - 10:00	Skouras E (FORTH)
	Demonstration of the use of an academic software: atomistic models of polymers	10:00 - 10:45	Mavrantzas V (FORTH)
	On the use of process scale software: fluid mechanics and process design	11:00 - 11:45	Fila V (Prague)
	<i>F. Modelling in Applications with Nanomaterials</i>		
	Nanofiltration and ultrafiltration modelling	12:15 - 13:00	Geraldes V (Lisbon)
Lunch			
	Modelling of atmospheric nanoparticles	15:00 - 16:00	Pandis S (Carnegie Mellon & FORTH)
	Modelling materials and transport in fuel cells	16:15 - 17:30	Weber A (Berkeley)
June 27, Friday			
	Modelling of membrane reactors and membrane contactors	09:00 - 10:00	Sanchez-Marcano J
	Transport phenomena in ion-exchange membranes during electrodialysis	10:15 - 11:00	Sistat P (CNRS)
	Conclusions – Discussion	11:00 - 11:30	Burganos V (FORTH)
	Payment of living expenses grant to attendants	11:30 - 16:00	