

Solvay Workshop on "Bridging the Gaps at the PCB Interface"

Multiscale Modelling in Physics, Chemistry & Biology

April 19-21, 2016
Programme

Tuesday April 19, 2016

08:30	09:15	REGISTRATION and starting Coffee	
09:20	09:30	<i>Welcome by Marc Henneaux (Director of the Solvay Institutes) and introduction by Jean-Pierre Boon (Université Libre de Bruxelles)</i> Chair: Jean-Pierre Boon	
09:30	10:05	Sauro Succi IAC-CNR Roma	Mesoscale modeling of complex moving matter across scales
10:05	10:40	Sumiyoshi Abe Mie University	Anomalous diffusion in volcanic seismicity
10:40	11:00	Ilya Karlin ETH Zürich	Mechanisms of droplet bouncing from micro-textured surfaces
11:00	11:20	<i>Coffee break</i>	
11:20	11:55	Rafael Delgado-Buscalioni Universidad Autonoma de Madrid	Combined strategies to climb up the scales in complex liquids simulations
11:55	12:30	Daan Frenkel University of Cambridge	Multi-scale modelling of self assembly
12:30	14:00	<i>Sandwich Lunch</i> Chair: Pierre Gaspard	
14:00	14:35	Hans Herrmann ETH Zürich	Packing of wires in cavities and growing surfaces
14:35	15:10	Alfons Hoekstra University of Amsterdam	Multiscale Modelling in Vascular Disease
15:10	15:30	Riccardo Rao University of Luxembourg	Nonequilibrium Thermodynamics of Chemical Reaction Networks
15:30	16:00	<i>Coffee Break</i>	
16:00	17:00	Solvay Lecture Raymond Kapral University of Toronto	Molecular Machines and Synthetic Motors: Active Motion on the Nanoscale
17:00		<i>Drink</i>	

Wednesday April 20, 2016

Chair: Raymond Kapral

09:30	10:05	Roberto Benzi Roma University	Statistical properties of Soft Glasses at the yield stress transition.
10:05	10:40	Kurt Kremer Max Planck Institute for Polymer Research	Multiscale Simulations for Soft Matter: Applications and New Developments
10:40	11:00	S. Kashif Sadiq Heidelberg Institute for Theoretical Studies	Towards multiscale spatiotemporal modeling of retroviral self-assembly
<i>11:00</i>	<i>11:20</i>	<i>Coffee Break</i>	
11:20	11:55	Caroline Lynn Kamerlin Uppsala University	Evolution Through Cooperativity in the Alkaline Phosphatase Superfamily
11:55	12:30	Peter Coveney University College London	Big Data Need Big Theory Too
<i>12:30</i>	<i>14:00</i>	<i>Group Photo and Sandwich Lunch</i>	
Chair: Peter Coveney			
14:00	14:35	James Lutsko Université libre de Bruxelles	Bridging length scales in the theory of nucleation
14:35	15:10	Simone Melchionna University "La Sapienza" Roma	Macromolecules and hydrodynamics: a simulation approach
15:10	15:30	Marco Lauricella Istituto per le Applicazioni del Calcolo-CNR	A Computational Study of Hydrate Methane Nucleation by Metadynamics
<i>15:30</i>	<i>16:00</i>	<i>Coffee Break</i>	
16:00	16:20	Josip Lovric University Lille	Molecular level study of Palmitic acid substrate on NaCl(100): physical phenomena of atmospheric interest
16:20	16:40	Pierre de Buyl KU Leuven	Self-propulsion through symmetry breaking
16:40	17:00	Agastya Prakash Bhati University College London	Computing ligand-protein free energies using multiscale methods
<i>17:15</i>	<i>Beer Party and Poster Session</i>		
<i>20:00</i>	<i>Conference Dinner at 'La Maison du Cygne' – Brussels Grand' Place</i>		

Thursday April 21, 2016

Chair: James Lutsko

09:30	10:05	Thomas Miller CALTECH	Computationally guided design of next-generation polymer electrolytes
10:05	10:40	Jesper Tegnér Karolinska University Hospital	On Bridging the Gap between Data and System Dynamics: Multi-omics Integrative Analysis of State-transitions in Cells and Data-driven formulation of System Equations
10:40	11:00	Alya Arabi Zayed University	Electric-Field Effects on the Double-Proton Transfer Reaction in Formic Acid Dimer
<i>11:00</i>	<i>11:20</i>	<i>Coffee Break</i>	
11:20	11:55	Nikolay Brilliantov University of Leicester	Generation of mechanical force by grafted polyelectrolytes in an electric field: Application to polyelectrolyte-based nano-devices.
11:55	12:30	Peter Wolynes Rice University	From Folding Proteins to Folding Chromosomes
12:30	14:00	<i>Sandwich Lunch</i>	
		Chair: Sauro Succi	
14:00	14:20	Fabrizio Pucci Université Libre de Bruxelles	More insight into protein thermal stability: from the molecular level to the analysis at the structuromic scale
14:20	14:40	Gianluca Di Staso University of Eindhoven	Hybrid MonteCarlo and lattice Boltzmann equation model for rarefied and non-rarefied gas flows
14:40	15:00	Robin Richardson University College London	Multiscale Modelling of Cerebral Blood Flow with lattice-Boltzmann for Clinical Decision-making
15:00	15:35	Pierre Gaspard Université libre de Bruxelles	Kinetics and thermodynamics of living copolymerization processes
15:35		Closing Remarks by Sauro Succi	