

Faraday Discussion 144: Multiscale Modelling of Soft Matter Programme

Monday 20 July 2009

11:00	Registration
13:00	Welcome and Introductions (Geertsema Hall, University of Groningen)
Session 1	Polymer simulation and coarse-graining methodologies Session Chairs: Michael P. Allen, <i>University of Warwick, UK</i> Doros N. Theodorou, <i>University of Athens, Greece</i>
13:15 Paper 1	Introductory Lecture Kurt Kremer* <i>Max Planck Institute for Polymer Research, Mainz, Germany</i>
14:15 Paper 2	Fine-graining without coarse-graining: an easy and fast way to equilibrate dense polymer melts Paola Carbone, Hossein Ali Karami-Varzaneh and Florian Müller-Plathe* <i>Technische Universität Darmstadt, Germany</i>
Paper 3	Systematic coarse-graining of molecular models by the Newton inversion Alexander Lyubartsev and Aatto Laaksonen* <i>Stockholm University, Sweden</i>
15:15	Afternoon Tea
15:45 Paper 4	Mesoscale modelling of polyelectrolyte electrophoresis Kai Grass and Christian Holm* <i>University of Stuttgart, Germany</i>
Paper 5	Kinetic Monte Carlo simulations of flow-induced nucleation in polymer melts Richard S Graham* and Peter D Olmsted <i>University of Nottingham, UK</i>
16:45	Close of Session
16:45 – 18:30	Poster Session (Spiegelzaal) <i>Kindly sponsored by Groningen Biomolecular Sciences & Biotechnology Institute</i>
19:15	Wine Reception (Venue TBC)
	There are plenty of restaurants around the town centre for delegates to make their own dinner arrangements.

Tuesday 21 July 2009

Session 2	Self-assembly, polymers and liquid crystals Session Chairs: Doros N. Theodorou, <i>University of Athens, Greece</i> Mark R. Wilson, <i>Durham University, UK</i>
09:00 Paper 6	Monte Carlo simulation of coarse grain polymeric systems Francois A Detcheverry, Darin Q Pike, Marcus Müller and Juan J De Pablo* <i>University of Wisconsin-Madison, USA</i>
Paper 7	A simple coarse-grained model for self-assembling silk-like protein fibers Marieke Schor, Bernd Ensing and Peter G Bolhuis* <i>University of Amsterdam, The Netherlands</i>
Paper 8	Phase behaviour of low-functionality, telechelic star block copolymers Federica Lo Verso*, Athanassios Z Panagiotopoulos and Christos N Likos <i>Johannes-Gutenberg-Universität Mainz, Germany</i>
10:30	Morning Coffee
11:00 Paper 9	Mesoscopic modelling of colloids in chiral nematics Miha Ravnik*, Gareth P Alexander, Julia M Yeomans and Slobodan Zumer <i>University of Ljubljana, Slovenia</i>
Paper 10	A molecular level simulation of a twisted nematic cell Matteo Ricci, Marco Mazzeo, Roberto Berardi, Paolo Pasini and Claudio Zannoni* <i>Università di Bologna, Italy</i>
Paper 11	Lyotropic self-assembly mechanism of T-shaped polyphilic molecules Andrew J Crane and Erich A Müller* <i>Imperial College London, UK</i>
12:30	Close of Session and Lunch/Posters (Spiegelzaal)

Tuesday 21 July 2009 cont.

Session 3	Colloids and Advances in Methodology Session Chairs: George Jackson, <i>Imperial College London, UK</i> Michael P. Allen, <i>University of Warwick, UK</i>
14:00 Paper 12	Coarse-grained simulations of charge, current and solvent flow in heterogeneous media Benjamin Rotenberg, Ignacio Pagonabarraga and Daan Frenkel* <i>University of Cambridge, UK</i>
Paper 13	Multi-particle collision dynamics simulations of sedimenting colloidal dispersions in confinement Adam Wysocki, C Patrick Royall, Roland G Winkler, Gerhard Gompper, Hajime Tanaka, Alfons van Blaaderen and Hartmut Löwen* <i>Heinrich-Heine-Universität Düsseldorf, Germany</i>
Paper 14	Can the isotropic-smectic transition of colloidal hard rods occur via nucleation and growth? Alejandro Cuetos, Eduardo Sanz and Marjolein Dijkstra* <i>Utrecht University, The Netherlands</i>
15:30	Afternoon Tea
16:00 Paper 15	Multi-scale simulation of asphaltene aggregation and deposition in capillary flow Edo S Boek*, Johan T Padding, Tom Headen and John Crawshaw <i>Schlumberger Cambridge Research, UK</i>
Paper 16	Coarse-graining dynamics for convection-diffusion of colloids: Taylor dispersion Jimaan Sané, Johan T Padding and Ard A Louis* <i>University of Oxford, UK</i>
Paper 17	Mori-Zwanzig formalism as a practical computational tool Carmen Hijon, Pep Español*, Erik Vanden-Eijnden and Rafael Delgado-Buscaloni <i>Universidad Nacional de Educacion a Distancia, Madrid, Spain</i>
17:30	Close of Session

19:30	Pre-Dinner Drinks (Het HeerenHuis, Groningen) Attendance by pre-booked ticket only
20:00	Conference Dinner (Het HeerenHuis, Groningen) Attendance by pre-booked ticket only

Wednesday 22 July 2009

Session 4	Membranes Session Chairs: D. Peter Tieleman, <i>University of Calgary, Canada</i> S.-J. Marrink, <i>University of Groningen, The Netherlands</i>
09:00 Paper 18	Hierarchical coarse-graining strategy for protein-membrane systems to access mesoscopic scales Gary S Ayton, Edward Lymon and Greg A Voth* <i>University of Utah, USA</i>
Paper 19	Towards and understanding of membrane-mediated protein-protein interactions Marianna Yiannourakou, Luca Marsella, Frédérick de Meyer and Berend Smit* <i>University of California, Berkeley, USA</i>
Paper 20	Measuring excess free energies of self-assembled membrane structures Yuki Norizoe, Kostas Ch Daoulas and Marcus Müller* <i>Georg-August-Universität, Germany</i>
10:30	Morning Coffee
11:00 Paper 21	Lateral pressure profiles in lipid monolayers Svetlana Baoukina, Siewert J Marrink and D Peter Tieleman* <i>University of Calgary, Canada</i>
Paper 22	Concerted diffusion of lipids in raft-like membranes Toukko Apajalahti, Perttu Niemelä, Praveen Nedumpully Govindan, Markus S Miettinen, Empu Salonen, Siewert J Marrink and Ilpo Vattulainen* <i>Tampere University of Technology, Finland</i>
Paper 23	Membrane poration by antimicrobial peptides combining atomistic and coarse grained descriptions Andrzej Rzepiela*, Durba Sengupta, Nicolae Goga and Siewert J Marrink <i>University of Groningen, The Netherlands</i>
12:30 Paper 24	Concluding Remarks Herman Berendsen* <i>University of Groningen, The Netherlands</i>
13:00	Acknowledgements
13:10	Close of Meeting