

Poster titles

Model lipid rafts at atomistic resolution: combining coarse-grained and all-atom MD simulations, **L. V. Schäffer, H. J. Risselada, A. J. Rzepiela, A. H. de Vries, S. J. Marrink**, *University of Groningen, The Netherlands*

Density imbalances and free energy of lipid transfer in supported lipid bilayers, **C. Xing and R. Faller**, *University of California Davis, USA*

Beyond amphiphiles: Coarse grained molecular dynamics simulation of star polyphiles, **J. J. K. Kirkensgaard and S. Hyde**, *Australian National University, Australia*

Coarse-grained simulations of α -helical peptides, **P. Gkeka and L. Sarkisov**, *University of Edinburgh, UK*

Systematic development of a coarse-grained model for 5CB (4-cyano-4'-pentylbiphenyl), **G. Megariotis, A. Vyrkou, A. Leygue and D. N. Theodorou**, *National Technical University of Athens, Greece*

Folding kinetics of an α -helix and a β -hairpin using coarse-grained simulations, **T. Bereau, D. Stone and M. Deserno**, *Carnegie Mellon University, USA*

Predicting porous organic polymers and networks: structures and properties, **A. Trewin and A. I. Cooper**, *University of Liverpool, UK*

Simulating self-assembled porous organic cages, **S. Jiang, A. Trewin and A. I. Cooper**, *University of Liverpool, UK*

FlowVRNano – a virtual laboratory dedicated to interactive simulation of large molecular systems, **N. Férey, O. Delalande and M. Baaden**, *Institut de Biologie Physico-Chimique, France*

Investigating bile salt aggregation using coarse-grained molecular dynamics, **A. Vila Verde and D. Frenkel**, *AMOLF-FOM Institute for Atomic and Molecular Physics, The Netherlands*

Hierarchical modelling of polymer permeation, **C. R. Herbers, D. Fritz, K. Kremer and N. F. A. van der Vegt**, *TU Darmstadt, Germany and Max Planck Institute for Polymer Research, Germany*

Precipitation of polycaprolactone nanoparticles *via* solvent-displacement: computational fluid dynamics modeling, **E. Gavi, D. L. Marchisio and A. A. Barresi**, *Politecnico di Torino, Italy*

Influenza HA fusion peptides favor stalk phases in MD simulations, **M. Fuhrmans and S. J. Marrink**, *University of Groningen, The Netherlands*

Encapsulation of local anesthetics into liposomes, **G. Guipponi and M. Pickholz**, *Universitat de Barcelona, Spain*

Coarse-grain modeling of lipid membrane adsorption on nanopatterned surfaces, **M. I. Hoopes, M. L. Longo and R. Faller**, *University of California, Davis, USA*

Effective coarse-grained potentials for DMPC-lipids by Inverse Monte Carlo method: Concentration dependence, **A. Mirzoev and A. Lyubartsev**, *Stockholm University, Sweden*

Determination of protein reduced electrostatic models from smoothed molecular electrostatic potentials, **L. Leherste and D. P. Vercauteren**, *University of Namur, Belgium*

Structure and dynamics of liquid water inside reverse micelles, **J. Martí, E. Guàrdia, J. Rodríguez and D. Iaria**, *Universitat Politècnica de Catalunya, Spain*

Hydrogen bonding and dynamic crossover in Polyamide-66: A molecular dynamics simulation study, **P. Carbone, H. A. Karimi Varzaneh and F. Müller-Plathe**, *University of Manchester, UK*

Back-mapping coarse-grained polymer models under sheared nonequilibrium conditions, **P. Carbone, X. Chen, G. Santangelo, A. Di Matteo, G. Milano and F. Müller-Plathe**, *University of Manchester, UK*

Excess entropy scaling of transport properties of Lennard-Jones chains, **T. Goel, C. Nath Patra, T. Mukherjee, M. Agarwal, R. Sharma, M. Parvez Alam and C. Chakravarty**, *Indian Institute of Technology-Delhi, India*

Agent-based modelling for molecular self-organization, **S. Fortuna and A. Troisi**, *University of Warwick, UK*

Multiscale modeling of polystyrene – Coarse graining methodology, **D. Fritz, V. Harmandaris, K. Kremer and N. F. A. van der Vegt**, *Max Planck Institute for Polymer Research, Germany*

Molecular dynamics study of non-ionic lipids at the air-water interface – structural aspects, **M. Velinova, S. Tzvetanov, A. Ivanova, Ph. Shushkov and A. Tadjer**, *University of Sofia, Bulgaria*

Hybrid particle-field molecular dynamics simulations for soft matter, **A. de Nicola, G. Milano, D. Roccatano and T. Kawakatsu**, *Università di Salerno, Italy*

Simulation studies of model systems for lung surfactant, **S. Baoukina, S. J. Marrink and D. P. Tieleman**, *University of Calgary, Canada*

Liquid crystallinity of the MARTINI coarse grained cholesterol model and its derivatives, **M. Yoneya**, *Nanotechnology Research Institute, AIST, Japan*

Comparison of a microgel simulation to a Poisson-Boltzmann cell model, **G. C. Claudio, C. Holm and K. Kremer**, *Max Planck Institute for Polymer Research, Germany*

Breaking CFTR into pieces: A coarse grained journey into putting together the pieces of the puzzle, **B. Nikolaidi and M. Sansom**, *University of Oxford, UK*

Toward coarse-grained simulations of block copolymers interaction with biological interfaces, **S. Hezaveh, G. Milano and D. Roccatano**, *Jacobs University Bremen, Germany*

Computer simulations of the interaction of fullerene with lipid membranes, **L. Monticelli, E. Salonen, P.-C. Ke and I. Vattulainen**, *INSERM, France and Helsinki University of Technology, Finland*

The counterion effect on the stability of structurally persistent micelles: MD simulations and experimental confirmation, **C. Jäger, H. Lanig, C. Böttcher, A. Hirsch and T. Clark**, *Friedrich-Alexander Universität Erlangen, Germany*

Added hexane controls the size and structure of structurally persistent micelles, **C. Jäger, M. Wildauer, H. Lanig, C. Böttcher, A. Hirsch and T. Clark**, *Friedrich-Alexander Universität Erlangen, Germany*

3D pressure field in lipid membranes and membrane protein complexes, **O. H. S. Ollila, H. J. Risselada, M. Louhivuori, A. Lamberg, A. Cattle, T. Vuorela, E. Lindahl, I. Vattulainen and S. J. Marrink**, *Tampere University of Technology, Finland*

The challenge of extracting atomistic and mesoscopic structural information from neutron diffraction measurement using EPSR, **R. Hargreaves**, *STFC, Rutherford Appleton Laboratory, UK*

Structure and charge transport in polymer semiconductors: Combined quantum, atomistic, and mesoscale modelling, **D. L. Cheung, D. P. McMahon and A. Troisi**, *University of Warwick, UK*

From achiral to chiral; a coarse-grained simulation study, **J. Lintuvuori and M. R. Wilson**, *Durham University, UK*

Discrete path sampling simulations of peptide folding, **J. M. Carr and D. J. Wales**, *University of Cambridge, UK*

Understanding complex protonation behaviour in mesoscale simulations using a dynamic, variable-dielectric Poisson-Boltzmann solver, **D. Eike, P. Verstraete, B. Murch, J. van Male and J. Fraaije**, *Brussels Innovation Center, The Procter & Gamble Company, Belgium*

Forced reptation revealed by chain pull-out simulations, **M. Bulacu and E. van der Giessen**, *University of Groningen, The Netherlands*

Bridging the scales of simulation and experiment: two scale characterisation of phospholipid bilayers, **A. H. de Vries, A.-P. Kunz, W. F. van Gunsteren and S. J. Marrink**, *University of Groningen, The Netherlands*

Quadrupolar defect structures generated by chiral islands in freely suspended smectic C films, **N. M. Silvestre, P. Patrício, M. M. Telo da Gama, A. Pattanaporkrattana, C. S. Park, J. E. MacLennan and N. A. Clark**, *Universidade de Lisboa, Portugal*

A hybrid molecular dynamics method with preserved Boltzmann distribution using coupling to a scaled thermostat, **N. Goga, A. J. Rzepiela, M. H. Louhivuori, H. J. C. Berendsen, A. H. de Vries and S. J. Marrink**, *University of Groningen, The Netherlands*

A coarse-grained model for a self-assembling dipeptide, **A. Villa, N. F. A. van der Vegt and C. Peter**, *Karolinska Institutet, Sweden*

Direct numerical simulations of colloidal dispersions: electrophoresis and non-linear rheology, **R. Yamamoto and T. Iwashita**, *Kyoto University, Japan*

Translation diffusivity and rotational relaxation in stratified mesophases, **G. Cinacchi and L. de Gaetani**, *University of Bristol, UK*

Mesophases of concave particles, **G. Cinacchi and J. S. van Duijneveldt**, *University of Bristol, UK*

Protein Domain Model – a preliminary exploration – Modelling the dynamics of a molecular machine, **L. Thøgersen**, *Aarhus University, Denmark*

Computer simulation studies of molecular order in chromonic mesophases, **F. Chami and M. R. Wilson**, *Durham University, UK*

Coarse grained modelling of self-assembling peptide fibres by Monte Carlo simulations, **T. Stedall and S. Hanna**, *University of Bristol, UK*

Conformational sampling of coarse grained peptide models, **O. Bezkorovaynaya, C. Peter and K. Kremer**, *Max Planck Institute for Polymer Research, Germany*

Lattice Boltzmann simulations of suspensions at multiple length scales, **R. G. M. van der Sman, F. Debask, G. Brans, J. Kromkamp, M. Vollebregt and R. M. Boom**, *Wageningen University, The Netherlands*

The Skinner Prize for the best poster was jointly awarded to Svetlana Baoukina of University of Calgary, Canada, for her poster on Simulation studies of model systems for lung surfactant and Juho Lintuvuori of Durham University, UK, for his poster From achiral to chiral; a coarse-grained simulation study.