CCP5 Annual General Meeting

10 – 12 September 2018

The University of Manchester

Programme

Day 1

13.00	Registration opens		
13.40	Welcome		

Session 1

Chair: **Carlos Avendaño**, The University of Manchester

13.45	**Fernando Escobedo**, Cornell University *Optimizing the Ordered Self-Assembly of Soft and Hard Nanoscale Building Blocks: Pure Components and Alloys*	–	35’ + 10’
14.30	**Massimiliano Chiappini**, Utrecht University *The role of particle curvature on twist, bend and splay deformations in nematic liquid crystals*	–	15’ + 5’
14.50	**Dwaipayan Chakrabarti**, University of Birmingham *Programming Hierarchical Self-Assembly of Patchy Particles into Colloidal Crystals via Colloidal Molecules*	–	15’ + 5’
15.10	Coffee Break	–	30’

Session 2

Chair: **Andrew Masters**, The University of Manchester

15.40	**Josep Bonet**, Rovira i Virgili University, Tarragona *Kinetic exchange of copolymer surfactants in micelles*	–	25’ + 5’
16.10	**Pablo de Castro**, King's College London *Phase separation dynamics of polydisperse colloids: a mean-field lattice-gas theory*	–	15’ + 5’
16.30	**David Quigley**, University of Warwick *Transport of Latent Heat in Seeded Nucleation Simulations*	–	15’ + 5’
16.50	**Karl Fairhurst**, Imperial College London *SAFT association potentials for MD simulations*	–	15’ + 5’
17.15	Poster Session and Drinks Reception		

Day 2

Session 3

Chair: **Fernando Escobedo**, Cornell University

09.00	**Francesco Sciortino**, Sapienza University *Collective Behavior of DNA made nanoparticles*	–	35' + 10'
09.45	**Carlos Avendaño**, The University of Manchester *Self-assembly of non-convex colloidal frames:* *The formation of lacuna ordered structures*	–	15' + 5'
10.05	**Daniel Corbett**, The University of Manchester *Dynamic Monte Carlos simulations of* *out-of-equilibrium colloidal liquid crystals*	–	15' + 5'
10.25	Coffee + Posters	–	30'

Session 4

Chair: **Karl Travis**, The University of Sheffield

10.55	**Carlos Nieto**, IFP Energies Nouvelles *Coarse-grained modeling of complex fluids and electrolytes.* *From parameterization to applications*	–	25' + 5'
11.25	**Martin Trusler**, Imperial College London *Thermophysical Properties and Phase Behaviour of Fluids* *for Application in Geological Carbon Storage*	–	25' + 5'
11.55	**Andrey Brukhno**, STFC, Daresbury Laboratory *Simulation of surfactants and lipids in solution:* *bridging between different scales and methods*	–	15' + 5'
12.15	Lunch	–	60'

Session 5

Chair: **Flor Siperstein**, The University of Manchester

13.15	**Peyman Moghadam**, University of Cambridge *The Role of High-Throughput Computational Screening* *in Materials Discovery*	–	25' + 5'
13.45	**Miguel Jorge**, University of Strathclyde *An accurate molecular model to predict adsorption of* *polar adsorbates in in metal organic frameworks with open metal sites*	–	15' + 5'
14.05	**Karen Johnston**, University of Strathclyde *Evaluation and Optimisation of Interface Force Fields* *for Water on Gold Surfaces*	–	15' + 5'

14.25	**Giuliana Giunta**, The University of Manchester *A Novel Coarse-Grained Model to Simulate High Molecular Weight Polymers in Contact with Solid Surfaces*	–	15’ + 5’
14.45	Coffee + Posters	–	30’

Session 6

Chair: **Francesco Sciortino**, Sapienza University

15.15	**Leo Lue**, University of Strathclyde *Structure and cluster formation in size asymmetric soft electrolyte systems*	–	15’ + 5’
15.35	**Paola Carbone**, The University of Manchester *Atomic characterization of the electrolyte/graphene interface*	–	15’ + 5’
15.55	**Simon Halstead**, The University of Manchester *The Effect of Halide Diffusion on the Liquid-Liquid Separation of Cobalt and Nickel Using Trihexyltetradecylphosphonium Halide Ionic Liquids*	–	15’ + 5’
16.15	**Martin Horsch**, American University of Iraq *Multicriteria optimization of pair potentials for bulk fluid properties and the vapour-liquid surface tension*	–	15’ + 5’
16.35	CCP5 Exec C/tee meeting		
19.15	Conference Dinner at Christie's Bistro		

Day 3

Session 7

Chair: **Josep Bonet**, University Rovira i Virgili, Tarragona

09.00	**Andrei Zvelindovsky**, University of Lincoln *Block copolymers in confinements and under external fields*	–	25' + 5'
09.30	**Gerardo Campos**, The University of Manchester *Coarse-grained potential derivation for modelling the self-assembly of block-copolymers in binary solvents*	–	15' + 5'
09.50	**Matthias Nébouy**, University of Lyon *Coarse-grained modelling of semicrystalline thermoplastic elastomers*	–	15' + 5'
10.10	**Javier Burgos**, University of Liverpool *Coarse-graining polymer semiconductors*	–	15' + 5'
10.30	Coffee Break	–	20'

Session 8

Chair: **Carlos Nieto**, IFP Energies Nouvelles

10.50	**Zengqiang Zhai**, University of Lyon *Molecular topology of semicrystalline polymers: simulation of mono and polydisperse systems*	–	15' + 5'
11.10	**Achille Giacometti**, University Ca' Foscari, Venice *The elixir phase of chain molecules*	–	15' + 5'
11.30	**Kostya Trachenko**, Queen Mary University of London *New understanding of collective modes and thermodynamics of the liquid and supercritical states*	–	15' + 5'
11.50	**Ivan Scivetti**, STFC, Daresbury Laboratory *Reorganization energy upon charging a single molecule on an insulator measured by atomic force microscopy*	–	15' + 5'
12.10	**James Shaw** *Hierarchical self-assembly of triblock patchy particles into a tetrastack lattice*	–	15' + 5'
12.30	Closing Remarks		

POSTER SESSION
Poster format should be A0 and in portrait orientation.

Velcro stickers for hanging posters will be provided. Posters may be set up during the lunch or coffee break on Monday. Posters can remain hanging to facilitate discussion during coffee breaks and lunch on Tuesday but should be taken down before the conference dinner on Tuesday evening as the boards will be removed on Wednesday morning.

The poster session will take place on Monday before the Drinks Reception and drinks and snacks will be provided.

List of Posters

1. Gerardo Campos-Villalobos, Jonatan Suaste, Andrew Haslam, George Jackson, Alejandro Gil-Villegas
   Molecular Thermodynamics of Adsorption Using a 2D-SAFT-VR-Mie Approach

2. Lauritz T. Bußfeld, Peter Behrens, Andreas M. Schneider
   Towards the coarse-grained modelling of dimethacrylate-based biomaterials

3. Malte Schäfer, Andreas M. Schneider, Peter Behrens
   Computational adaptation of metal-organic frameworks for highly selective sensor materials

4. Pallabi Haldar, Flor Siperstein, Alessandro Patti
   Modelling the kinetics of silica polymerization

5. Jezabel Boni, Paola Carbone, Robert Dryfe, Anne Juel
   Modelling of Electrowetting and Other Interfacial Properties of Liquids on Graphene

6. Emma L. Wood, Nigel Clarke
   Predicting phase separation in polymer blends that contain branched molecules

7. R. Sharpe, D. Case, A. McSloy, E. Dashjav, F. Tietz, P. Panchmatia
   Structure and Dynamics of Li-rich $Li_{1+x}Al_xTi_{2-x}(PO_4)_3$ (LATP), where $0.3<x<0.5$: A Combined Computational and Experimental Study

8. Kristina Sladekova, Christopher Campbell, Miguel Jorge
   The Effect of Atomic Point Charges on Adsorption Isotherms of Metal Organic Frameworks

9. José J. Burgos-Mármol, Annalaura Del Regno, Flor Siperstein, Alessandro Patti
   Rheological consequences of the addition of Janus nanodimers to a lamellar phase

10. Ian Shuttleworth
    Development of the ReaxFF Reactive Force-Field Description of Gold Oxides

11. Idil Ismail, Aliya Shafiq, Rafi Mahmood, Nissar Aziz, Anna Akinshina, Michael Seaton
    Interactions of terpenes in water and aqueous alcohol solutions

12. José J. Burgos, O. Álvarez-Machancoses, Alessandro Patti
    Modeling the effect of chain stiffness on the behaviour of polymer nanocomposites

13. Charlie Wand, Paola Carbone, Andrew Masters
    Calculating the scission free energy of worm-like micelles using dissipative particle dynamics simulations

14. Olivia Nile Sobek, Miguel Jorge
    Assessing coarse-grained models for the self-assembly of block copolymers

15. David J Bray, Annalaura Del Regno, Richard L. Anderson
    Bridging the gap between in-silico and experimental chemistry – a close view into the formulation world
16. Sara Fortuna, Rengin Pekoz, David L. Cheung, Davide Donadio, Karen Johnston
    Phase behaviour of self-assembled monolayers controlled by tuning physisorbed and chemisorbed states

17. Mitha Al Jabri, Laura Najem, and Thomas L. Rodgers
    Dissolution of Surfactant Lamellar Phases

18. Maud Formanek, Lorenzo Rovigatti, Emanuela Zaccarelli and Angel Moreno
    From single-chain nanoparticles to gels: Computational study of the competition between intra- and inter-molecular bonding of polymers in solution

19. Francesco Pelizza and Karen Johnston
    Computational modelling of the effect of surfaces on polyvinyldenedifluoride

20. Michael F. Faulkner, Liang Qin, A. C. Maggs, and Werner Krauth
    Rejection-free Markov-chain Monte Carlo in liquid water