CCP5 Annual General Meeting

Materials Modelling: Simulation Meets Experiment

Technology and Innovation Centre, University of Strathclyde, Glasgow

11-13 September 2017

Monday 11th September

11:00	**REGISTRATION AND LUNCH**
12:30	**Welcome**
CHAIR: Paul Mulheran	
12:35	**FRIEDRICH KREMER (35 + 10 minutes)** *Molecular dynamics at nanometric length scales*
13:20	**Jose-Javier Burgos-Marmol (15 + 5 minutes)** *Molecular dynamics of polymer nanocomposites*
13:40	**Francesco Pelizza (15 + 5 minutes)** *Multiscale Modelling of PVDF bulk and surface-interface physical properties*
14:00	**Olga Guskova (15 +5 minutes)** *Synthesis and characterization of crystalline phases of small-molecule semiconductors and in silico estimation of their charge carrier mobility*
14:20	**COFFEE BREAK AND POSTER SETUP** (30 minutes)
CHAIR: Alessandro Patti	
14:50	**BILL MACDONALD (25 + 5 minutes)** *Polyester Films-Can You Teach An Old Dog New Tricks?*
15:20	**Angelo Bongiorno (15 +5 minutes)** *Structure and Mechanical Properties of Pristine and Oxidized Epitaxial Graphene Films: Experiments and DFT calculations*
15:40	**Peter Brommer (15 +5 minutes)** *2d molecular dynamics study of substrate-dependent growth of graphene on copper*
16:00	**Karina Kubiak-Ossowska (15 + 5 minutes)** *Negatively Charged Protein Adsorption to Negatively Charged Surface*
16:20	**POSTER SESSION with coffee/tea and snacks**
18:00	**WINE RECEPTION, Glasgow City Chambers**

Tuesday 12th September

CHAIR: Joop ter Horst	
09:00	**DOROTHY DUFFY (35 + 10 minutes)** *Laser induced melting of metallic films: Modelling meets experiment*
09:45	**Andrew McCluskey (15 + 5 minutes)** *Simulations to understand reflectivity: how coarse can we go?*
10:05	**Stephen Skowron (15 + 5 minutes)** *Electron-beam induced chemistry of organic molecules*

10:25	**Alessandro Patti – CCP5 AGM 2018 organiser**
10:30	**COFFEE BREAK** (40 minutes)
CHAIR: Pooja Panchmatia	
11:10	**Andrey Brukhno (15 + 5 minutes)** *Supported lipid films under a varying electric field: modelling a voltammetry molecular sensor*
11:30	**Stephen Yeandel (15 +5 minutes)** *Lithium Diffusion in Complex Phosphidosilicate Materials*
11:50	**Christian Lorenz (15 + 5 minutes)** *Investigating the interfacial properties and aggregation of bile salts*
12:10	**Carlos Ferreiro-Rangel (15 + 5 minutes)** *Prediction of binary SALR + SA fluid phase behaviour by means of Density Functional Micelle Theory Calculations*
12:30	**Neil Allan - CCP5 chair** (10 minutes)
12:40	**BUFFET LUNCH** (1 hour)
CHAIR: Colin Freeman	
13:40	**AMY ROBERTSON (25 + 5 minutes)** *Crystallisation Process Development: Past, Present and Future*
14:10	**Joao Coutinho (15 +5 minutes)** *Hydrotropic solubilization of hydrophobic compounds in aqueous solutions of ionic liquid*
14:30	**Sebastien Lectez (15 +5 minutes)** *Simulation of Complexation of Rare Earth Elements in Aqueous Chloride Solutions.*
14:50	**Andrew Milne (15 + 5 minutes)** *Transferable Force Field Parameterisation of Organosilicates Using Multiscale Modelling*
15:10	**COFFEE BREAK** (30 minutes)
CHAIR: Dorothy Duffy	
15:40	**Ateeque Malani (15 + 5 minutes)** *Understanding self assembly of silica precursors using Monte Carlo Simulations*
16:00	**Tom Underwood (15 + 5 minutes)** *Phase diagrams of molecular solids_from lattice-switch Monte Carlo in DL_MONTE*
16:20	**Colin Freeman (15 + 5 minutes)** *The influence of amino acids on amorphous calcium carbonate structure and formation*
16:40	**JOOP TER HORST (35 + 10 minutes)** *Crystal Nucleation of Small Organic Molecules*
17:25	**Poster collection**
18:30	**CONFERENCE DINNER, 29 Glasgow**

Wednesday 13th September

CHAIR: Miguel Jorge	
09:00	**PETER MONSON (35 + 10 minutes)** *Molecular theory and simulation of the dynamic behavior of fluids confined in mesoporous materials*

09:45	**Richard Gowers (15 + 5 minutes)** *Benchmarking of GCMC simulation programs in application to gas adsorption*
10:05	**Christopher Williams (15 + 5 minutes)** *Ion Permeation in Graphene Oxide Membranes: A molecular simulation perspective*
10:25	**COFFEE BREAK** (20 minutes)
CHAIR: Peter Brommer	
10:45	**Jose Gomes (15 + 5 minutes)** *Molecular dynamics simulations of Zn-Al layered double hydroxides with different intercalated ions*
11:05	**Edward Jackson (15 + 5 minutes)** *Quantify energetic barriers to the diffusion of C8 aromatics in porous organic cages*
11:25	**DARREN BROOM (25 + 5 minutes)** *Gas adsorption by nanoporous materials: Experimental challenges and the role of computational modelling and simulation*
11:55	Closing remarks
	LUNCH

DL SOFTWARE WORKSHOP

Wednesday 13th	14:00-17:00	CW404b
Thursday 14th	09:00-17:00	CW404b
Friday 15th	09:00-17:00	CW404b

POSTER SESSION

Poster format should be (maximum) **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 Civic Reception and drinks and snacks will be provided.

A prize will be awarded for the best poster presentation.

LIST OF PARTICIPANTS

Nasser Afify	Institute of Materials and Processes, University of Edinburgh, UK	N.Afify[AT]ed.ac.uk	-
Lorenzo Agosta	Department of Materials and Environmental Chemistry, Stockholm University, Sweden	lorenzo.agosta[AT]mmk.su.se	Poster
Mohammed Al Qaraghuli	Department of Chemical and Process Engineering, University of Strathclyde, UK	mohammed.al-qaraghuli[AT]strath.ac.uk	-
Neil Allan	School of Chemistry, University of Bristol, UK	n.l.allan[AT]bris.ac.uk	-
Andrew Bell	Department of Chemical and Process Engineering, University of Strathclyde, UK	a.bell[AT]strath.ac.uk	Poster
Angelo Bongiorno	Nanoscience Initiative, City University of New York, USA	angelo.bongiorno[AT]csi.cuny.edu	Talk
Peter Brommer	School of Engineering, University of Warwick, UK	p.brommer[AT]warwick.ac.uk	Talk
Darren Broom	Hiden Isochema Ltd, UK	dbroom[AT]hidenisochema.com	Invited Talk
Andrey Brukhno	Scientific Computing Department, STFC, UK	andrey.brukhno[AT]stfc.ac.uk	Talk/Poster
Jose-Javier Burgos-Marmol	School of Chemical Engineering and Analytical Science, The University of Manchester, UK	josejavier.burgos-marmol[AT]manchester.ac.uk	Talk
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João A.P. Coutinho	Department of Chemistry, University of Aveiro, Portugal	jcoutinho[AT]ua.pt	Talk
James Denholm	Department of Physics, University of Strathclyde	j.denholm[AT]strath.ac.uk	-
Dorothy Duffy	Department of Physics, University College London	d.duffy[AT]ucl.ac.uk	Invited Talk
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	STFC, UK		
Jose Gomes	Department of Chemistry, University of Aveiro, Portugal	jrgomes[AT]ua.pt	Talk
Richard Gowers	School of Engineering, University of Edinburgh, UK	richard.gowers[AT]ed.ac.uk	Talk
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	Liverpool, Daresbury Laboratory, Sc. Tech., UK		
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