The eSSENCE Multiscale Materials Modelling Meeting 2014

(schedule version 30th of May 2014)

Monday 2nd of June

Room Days 1 and 2: Häggsalen at the Ångström laboratory

Time	Speaker	Title
13.00-13.15	Kersti Hermansson (Organiser)	*Welcome*
13.15-13.45	Roland Lindh (UU)	*"Chemiluminescence"*
13.45-14.15	Alexander Lyubartsev (SU)	*"Systematic Coarse-Graining of Molecular Models by Inverse Monte Carlo"*
14.15-14.45	Magnus Ullner (LU)	*"Simulations of Osmotic Pressure in Polyelectrolyte Solutions"*
14.45-15.00	Mikaela Lindgren (CTH)	*"Oxidation of Zirconium Alloys by Water: Anode, Cathode and Transport Properties"*
15.00-15.30	*Coffee*	
15.30-15.50	Ingela Nyström (UU)	*"About the eSSENCE Programme"- from the eSSENCE Coordinator*
15.50-16.20	Sten Sarman (SU)	*"Thermomechanical Coupling in Liquid Crystals"*
16.20-16.50	Ran Friedman (LNU)	*"Modelling Biomaterials –Phenomenological Coarse Grained Models versus Atomistic Representation"*
16.50-17.20	Vincenzo Carravetta (CNR, Pisa)	*"Surface Effects in Electron Photoemission from Solutions: Cysteine in Water"*
17.20-17.50	David van der Spoel (UU)	*"Towards Accurate Thermodynamics Calculations for Liquids"*
17.50-18.30	*Poster Presentations*	
18:30-19.30	*Posters & Mingle*	
19.30-	*Buffet Supper at the Ångström Laboratory*	

Tuesday 3rd of June – Quality Day – in collaboration with the European Modelling Council

Time	Speaker	Title
09.00-09.30	Per Hyldgaard (CTH)	*"Consistent Exchange-van der Waals Density Functional: Facing the Challenge of Competing Interactions"*
09.30-10.30	Anthony Reilly (Cambridge Crystallographic Data Centre)	*"Crystal-Structure Prediction – Blind Tests, Progress and Challenges"*
10.30-11.00	*Coffee*	
11.00-12.00	Lennart Lindfors (AstraZeneca R&D)	*"In Silico Prediction of Drug Solubility – Does It Work?"*
12.00-13.00	*Lunch*	
13.00-13.15	Johan Tysk (UU)	*Comments from the Faculty of Science and Technology at Uppsala University*
13.15-13.30	Kersti Hermansson (Organiser)	*"Materials Modelling from a National and European Perspective"*
13.30-14.30	Michele Parrinello (ETH)	*"Challenges and Perspectives in Computational Materials Modelling"*
14.30-15.00	Hans Ågren (KTH)	*"Quantum Mechanics–Capacitance Molecular Mechanics for Molecules in Heterogeneous Environments"*
15.00-15.30	Philippe Bopp (Bordeaux U)	*"Combining Interaction Models is Not Without Danger"*
15.30-16.00	*Coffee*	
16.00-16.30	Aatto Laaksonen (SU)	*"Modelling Ionic Liquids – a Potential Source of Headache"*
16.30-17.30	Sven Lidin (LU)	*"Why Better Experimental Data Needs More Modelling"*
17.30-18.30	*Panel Discussion*	
19.30-	*Dinner Downtown*	

Wednesday 4th of June

Room: Å2005 at the Ångström laboratory

Time	Speaker	Title
09.00-09.30	Michael Probst (Innsbruck U)	*"Computational Materials Science for the ITER Reactor"*
09.30-10.00	Itai Panas (CTH)	*"Phonon Mediated Local–Nonlocal Charge Redistribution in Oxide Superconductors"*
10.00-10.30	Laurent Proville (CEA-Saclay)	*"Atomic-Scale Modelling of Plastic Deformation for Model Materials: An Evidence for Low Temperature Quantum Effect"*
10.30-11.00	*Coffee*	
11.00-11.30	Anna Delin (KTH)	*"Spin Dynamics and Spin Caloritronics – Recent Development"*
11.30-11.45	Matti Hellström (UU)	*"Odd Cu Clusters on ZnO Become Positive – but Even Don't!"*
11.45-12.15	Per Linse (LU)	*"Virus Self-Assembly Induced by Polyions"*
12.15-12.30	Alexander Kaiser (Innsbruck U)	*"Vacancy Controlled Self-Assembly of Fullerenes on Metal Surfaces"*
12.30	*Close of Conference*	