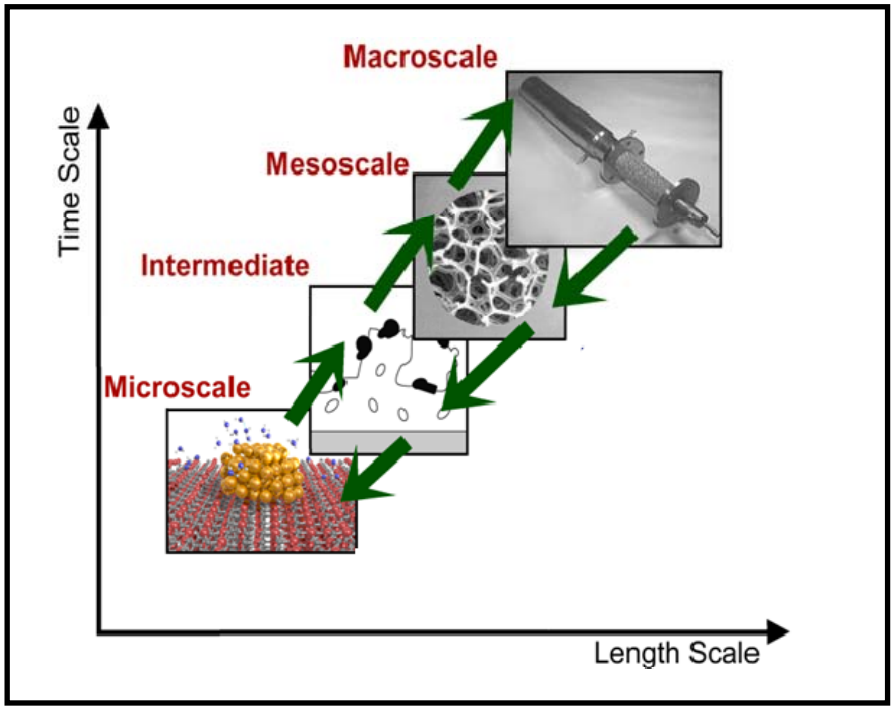
Multiscale Materials Modelling Meeting
and
QUALITY of Materials Modelling Symposium

arranged in co-operation with the 'Advanced materials and nanotechnologies' unit of the European Commission



The Ångström Laboratory, Uppsala University, Sweden
2^{nd} – 4^{th} June 2014

Local Organiser: Kersti Hermansson

Notes

Monday 2nd June

Oral presentations will take place in Häggsalen

11.30 – 13.00	Registration and Light Lunch	
13.00 – 13.15	Welcome and Information (Kersti Hermansson)	

Session One

Session Chair: Pavlin Mitev

13.15 – 13.45	Roland Lindh Uppsala University	*Chemiluminescence*
13.45 – 14.15	Alexander Lyubartsev Stockholm University	*Systematic Coarse-Graining of Molecular Models by Inverse Monte Carlo*
14.15 – 14.45	Magnus Ullner Lund University	*Simulations of Osmotic Pressure in Polyelectrolyte Solutions*
14.45 – 15.00	Mikaela Lindgren Innsbruck University	*Oxidation of Zirconium Alloys by Water: Anode, Cathode and Transport Properties*
15.00 – 15.30	Coffee	

Session Two

Session Chair: Francesca Mocci

15.30 – 15.50	Ingela Nyström Uppsala University	*About the eSSENCE Programme*
15.50 – 16.20	Vincenzo Carravetta CNR, Pisa	*Surface Effects in Electron Photoemission from Solution: Cysteine in Water*
16.20 – 16.50	Ran Friedman Linnæus University	*Modelling Biomaterials – Phenomenonological Coarse Grained Models versus Atomistic Models*
16.50 – 17.20	Sten Sarman Stockholm University	*Thermomechanical Coupling in Liquid Crystals*
17.20 – 17.50	David van der Spoel Uppsala University	*Towards Accurate Thermodynamics Calculations for Liquids*
17.50 – 18.30	Oral Poster Advertisements (Chaired by Matti Hellström)	
18.30 – 19.30	Poster and Mingling Session	
19.30 –	Buffet Dinner at Cafe Ångström	

Tuesday 3rd June – QUALITY of Materials Modelling

arranged in co-operation with the European Materials Modelling Council
of the 'Advanced materials and nanotechnologies' unit (EC)

Oral presentations will take place in Häggsalen

Session One

Session Chair: Kersti Hermansson

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 CCDC, Cambridge	*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 at Cafe Ångström	

Session Two

Session Chair: Peter Broqvist

13.00 – 13.15	Johan Tysk Uppsala University	*Comments from the Faculty of Science and Technology at Uppsala University*
13.15 – 13.30	Kersti Hermansson Uppsala University	*The Materials Modelling Council – a European initiative* within the *Advanced materials and nanotechnologies* unit of the EC
13.30 – 14.30	Michele Parinello ETH, Zurich	*Challenges and Perspectives in Computational Materials Modelling*
14.30 – 15.00	Philippe Bopp Bordeaux University	*Combining Interaction Models is Not Without Danger*
15.00 – 15.30	Coffee	

Session Three

Session Chair: Olav Vahtras

15.30 – 16.00	Hans Ågren KTH, Stockholm	*Quantum Mechanics – Capacitance Molecular Mechanics for Molecules in Heterogeneous Environments*

16.00 – 16.30	Aatto Laaksonen Stockholm University	*Modelling Ionic Liquids – a Potential Source of Headache*
16.30 – 17.30	Sven Lidin Lund University	*Why Better Experimental Data Needs More Modelling*
17.30 – 18.30	Panel Discussion	
19.30	Dinner at Åbar in Central Uppsala	

Wednesday 4th June

Oral presentations will take place in Å2005

Session One

Session Chair: Marcus Lundberg (Uppsala University)

09.00 – 09.30	Michael Probst Innsbruck University	*Computational Materials Science for the ITER Reactor*
09.30 – 10.00	Itai Panas CTH, Gothenburg	*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	

Session Two

Session Chair: Matthew Wolf (Uppsala University)

11.00 – 11.30	Anna Delin KTH, Stockholm	*Spin Dynamics and Spin Caloritronics – Recent Development*
11.30 – 11.45	Matti Hellström Uppsala University	*Odd Cu Clusters on ZnO Become Positive – but Even Don't!*
11.45 – 12.15	Per Linse Lund University	*Virus Self-Assembly Induced by Polyions*
12.15 – 12.30	Alexander Kaiser Innsbruck University	*Vacancy Controlled Self-Assembly of Fullerenes on Metal Surfaces*
12.30	Closing Comments (Kersti Hermansson)	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