eSSENCE Multiscale Modelling of Materials (and Molecules) 2015

All sessions are in Häggsalen at the Ångström Laboratory

Monday 8 June

(version 5 June2015)

13.00-13.10	Kersti Hermansson	Welcome and Introduction
Session 1: **"From fine-grained ..."**		**Chair: Hans Ågren (KTH)**
13.10-14.00	*Keynote talk:* Lars Ojamäe (LiU)	"*Modelling at the electronic and atomistic scales: From water clusters to inorganic materials*"
14.00-14.30	Per Hyldgaard (CTH)	"*Role of spin in the Van der Waals density functional* "
14.30-15.00	Anders Bergman (UU)	"*Modelling chiral magnets - from individual atoms to collective excitations*"
15.00-15.20	Joakim Halldin Stenlid (KTH)	"*On the origin of hydrogen gas evolution from copper in anoxic water*"
15.20-15.45	*Coffee*	
Session 2: **" ..to more coarse-grained and large-scale"**		**Chair: Olle Eriksson (UU)**
15.45-16.35	*Keynote talk:* Pietro Asinari (Torino)	"*Modelling beyond the atomistic scale: From molecular interfaces to open issues in renewable energy engineering*"
16.35-17.05	Jolla Kullgren (UU)	"*Parameterized methods for accurate simulations of metal oxide surfaces*"
17.05-17.25	Björn Dahlgren (KTH)	"*Modelling interfacial radiation chemistry without explicit atoms or electrons*"
17.25-17.45	Jacinto Sa (UU)	"*Shining light into chemistry's dark secrets: from experiment to theory*"
Session 3: **"Poster session – oral & traditional"**		**Chairs: Ali Rafieefar, Dou Du, Getachew Kebede (UU)**
17.45-18.30	*5 min break, and then Oral POSTER presentations*	
18.30-19.30	*Poster session & mingel*	
19.30-	*Buffet at the Café Ångström*	

Tuesday 9 June

Session 4: **"Dynamics"**		**Chair: Magnus Ullner (LU)**
09.00-09.50	*Keynote talk:* David Sumpter (UU)	"*The principles of collective fish behaviour – are there similarities to molecular dynamics*?
09.50-10.20	Joakim Stenhammar (LU)	"*Phase behaviour of active Brownian particles*"
10.20-10.40	Håkan Hugosson (KTH)	"*Quantum Molecular Dynamics studies of polymer-based thermoelectric materials*"
10.40-11.10	*Coffee*	
Session 5: **"Modelling challenges of biosystems"**		**Chair: Peter Broqvist (UU)**
11.10-12.00	*Keynote talk:* Per Siegbahn (SU)	"*How to solve an important chemical problem for a large system by quantum chemical methods: The case of oxygen formation in photosynthesis*"
12.00-12.30	Murugan Arul (KTH)	"*Multiscale modeling approaches for Diagnostic Probes Design*"
12.30-13.30	*Lunch*	
Session 6: **"Biosystems II"**		**Chair: Mårten Ahlqvist (KTH)**
13.30-13.50	Ingela Nyström (UU)	"*The eSSENCE program*"
13.50-14.20	Fernanda Duarte (UU)	"*Understanding Functional Evolution in the Alkaline Phosphatase Superfamily*"
14.20-14.40	Xianqiang Sun (KTH)	"*Theoretical Studies of G-Protein-Coupled Receptors*"
14.40-15.00	Stefan Knippenberg (KTH)	"*An exploration of ADC data to describe non-linear properties of cyanine molecules*"
15.00-15.30	***Discussion*** *(with coffee)* ***– what do we need?*** *(Kersti Hermansson)*	

Poster presentations

Abas	Mohsenzadeh Syouki	"*The water gas shift reaction on nickel facets: A comparative DFT study*"
Rafael	Couto	"*Resonant Inelastic X-ray Scattering of gas phase water*"
Ignat	Harczuk	"*Generalized Frequency Dependent Polarizabilities and Hyperpolarizabilities in Extended Molecular Mechanical Systems*"
Rocio	Marcos	"*Theoretical investigation of the iron-catalyzed hydrogenation of bicarbonated to formate*"
Amina	Mirsakiyeva	"*Quantum Molecular Dynamics Studies of Thermoelectric Polymer Systems*"
Daniel	Mårtensson	"*Molecular Dynamics Investigations of Water Oxidation I2M Reaction*"
Yan	Wang	"*Molecular Adhesion at Clay Nanocomposite Interfaces Depends on Counterion Hydration - Molecular Dynamics Simulation of Montmorillonite/Xyloglucan*"
Dou	Du	"*Oxygen Storage in Nanoceria: A Revisit by Employing Hybrid Density Functionals*"
Erik	Källman	"*Quantum chemical tools for orbital-specific interpretation of x-ray processes*"
Esko	Makkonen	"*Theoretical study of water-oxidizing complexes with iron center*"
Anik	Sen	"*Computational Crystallography of water*"
Matthew	Wolf	"*Formation of superoxides at fluorine doped ceria surface facets*"
Changgang	Xu	"*Purification and quantification of antibody IgG with DNA-nanocellulose composite membrane*"
Getachew	Kebede	"*A Van der Waals density functional study on the structure and energetics of H_2O/NaCl(100) and H_2O/MgO(100) interfaces*"