Program **Version 6 June 2012**

Thursday 7 June (room Å2005)		
11.30		Registration starts and sallad lunch available (Outside room Å 2001 and in room Å 2004)
13.15	.le. 15 min	Introduction and Welcome, Prof. Kersti Hermansson (room Å2005)
13.30	20 + 10 min 20 + 10 min	At the bottom: *The quantum region* Prof. Per Hyldgaard (Chalmers): *Dispersion interactions in DFT calculations* Prof. Hans Ågren (KTH, SeRC): *Beyond periodic DFT*
14.30	30 + 10 min	Medium range: *Ab initio-based force fields from a Neural Network approach* (Dr. Jörg Behler, Ruhr-Universität Bochum, Germany)
15.10	35 min	*Photo session + Coffee*
15.45	10 + 5 min	*The eSSENCE program* (Prof. Ingela Nyström, eSSENCE coordinator)
16.00	30 + 10 min	At the top: *Micro-kinetic modelling and computational fluid dynamics* (Prof. Bengt Andersson, Chalmers)
16.40	50 min	3-minute oral poster presentations (if you want to show sth on the computer - give to Pavlin Mitev beforehand) Lars Ojamäe (LiU) *Colloidal GaN Quantum Dots* Pooria Farahani (UU) *CASPT2 computations on medium- to large-size systems: the "lovCASPT2" approach* Henrik Löfås (UU) *Conductance traces over a wide range of geometries by ab initio molecular dynamics simulations* Daniel Roca-Sanjuán (UU) *CASPT2 computations on medium- to large-size systems: the orbital-free embedding method* Baochang Wang (UU) E*lectronic structure of high pressure phases TiO_2: A hybrid functional and GW method's study* Bogdan Frecus, Zilvinas Rinkevicius, Jacob Kongsted (KTH) *Multiscale modeling of EPR parameters of spin-labels in complex environments* Lars Bergqvist, A. Bergman, A. Taroni, C. Etz and O. Eriksson (KTH and UU) *Magnon properties in magnets from atomistic spin dynamics* Yunguo Li (UU) *Metal-decorated GO for gas adsorption and strain effect* Jolla Kullgren, P. Broqvist, P. Mitev, Ch. Castleton, K. Hemansson (UU) *Ceria chemistry* Petter Persson, Tomas Österman, Svante Hedström, Marta Knitter, Hannes Kuusisto(LU): *Nanoenergy Calculations* Per Linse and Gunnar Karlstrom (LU): *Dipolar order in molecular fluids* Tommaso Casalini (Milano, UU) *Molecular modeling of agar/carbomer hydrogels*
17.30	60-75 min	Panel discussion with refreshments How far are we - what can we do? Do software and hardware developments go hand in hand? How can we get more of e-science into the undergraduate curriculum? Panel members: P. Hyldgaard+ H. Ågren + J. Behler + B. Andersson + Bo Jönsson + Lars Pettersson
18.45	At the latest	*For those who have hotel rooms: Taxis will take you downtown.*
20.00		*Dinner at Saluhallen: resturang Åbar (see map on the conference webpage)*
Friday 8 June (Room Å2005)		
9.00	100 min 15+ 5 min each	Invited and contributed talks from the participants Jean-Francois Boily (UmU): *Coupling theory to experiment for mineral surfaces* Axel Thuresson (LU): *Monte Carlo simulations concerning the tactoid formation of charged clay platelets* V.Veryazov (LU): *Disordered calcium silicates. Is there any use for quantum chemistry?* Marcus Lundberg (UU): *Multiscale enzyme modeling inspired by materials theory*

		Anton Grigoriev (Physics&Astronomy, UU) *Quantum chaos signatures in the conductance histograms of the molecular electronic devices.*
10.40	30 min	*Coffee and poster session*
11.10	80 min = 15+ 5 min each	Invited and contributed talks from the participants Peter Broqvist (Materials Chemistry, UU) : *Understanding oxide interfaces through core-level shifts.* Itai Panas (Chalmers): *Atomistic Divide and Conquer Paradigm for High-Tc Superconductivity* S. Borlenghi (KTH): *Manipulating the magnetization with heat and current: simulation techniques for realistic devices* Zilvinas Rinkevicius (KTH): *QM/MM methods for EPR parameters of radicals*
12.20	10 min	Roundup
12.30		*Sandwich (nice) lunch*