To push the boundaries of e-science closer to realistic applications, development of methods and models at all levels is needed, from the electronic scale to coarse-grained simulations**.** In particular, we must find ways to combine methods in a powerful and creative fashion to bridge the different time and length gaps in a seamless fashion. The national e-science programme eSSENCE – where *Uppsala University*, *Lund University* and *Umeå University* are partners – now welcomes you to the meeting

"Multiscale materials modelling"

at the Ångström Laboratory, Uppsala University
7 -8 June (two half-days) 2012

http://essenceofescience.se/materials-2012/

At this meeting, we will discuss the challenges of multiscale modelling, as well as a number of interesting examples of modern materials and molecular simulations. We will use the word "materials" in a broad sense, i.e. also including molecules and molten materials (liquids). Colleagues from our national sister program SeRC, as well as all other e-science actors or interested colleagues are welcome to attend the meeting. Senior researchers, postdocs and PhD students are all equally welcome.

Scientific contributions: Four external speakers will give plenary lectures on Day 1. Posters will be accompanied by short oral poster presentations - you are most welcome to sign up to present a poster! See further info on the web. There will also be invited and contributed 15-minute oral presentations (+ discussion). See further info on the web.

Registration: The meeting and the dinner and lunch will be *free of charge to registered participants.* Participants from outside Uppsala who need hotel accommodation will receive it free of charge. Sign up for the meeting by sending an e-mail to Dr. Pavlin Mitev (pmitev@kemi.uu.se) with some information as described on the web *http://essenceofescience.se/materials-2012/.* Do this before 25 May! If you need accomodation - tell us as soon as possible and preferably before 16 May!

***Information and questions*:** Contact Kersti Hermansson (kersti@kemi.uu.se).

EXCERPT FROM THE PROGRAM FOR THURSDAY, 7 JUNE 2012 (DAY 2 IS ON THE WEB!)

13.15	Introduction and welcome, Prof. Kersti Hermansson
13.30	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	Medium range: *Ab initio-based force fields from a Neural Network approach* (Dr. Jörg Behler, Ruhr-Universität Bochum, Germany)
15.30	*The eSSENCE program* (Prof. Ingela Nyström, eSSENCE coordinator)
15.45	At the top: *Micro-kinetic modelling and computational fluid dynamics* (Prof. Bengt Andersson, Chalmers)
16.30	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?
17.45	Oral poster presentations.
20.00	*Dinner downtown*

W-E-L-C-O-M-E !