Report from the eSSENCE-EMMC meeting "Multiscale modelling of materials and molecules 2022"

The eSSENCE-EMMC Multiscale materials modelling meeting 2022 was held on-site at Uppsala University 1-3 June 2022. Participants came from Austria, Belgium, France, Germany, Italy, Norway Poland, Spain, Sweden, UK, and USA. Altogether there were 85 registered particpants.

All speakers, international and national, participated on-site except Dr Ansgar Schäfer from BASF (DE).

Multiscale modelling (coupling & linking of models) as well as ***digitalization*** and the ***hybridization of physics-based and data-driven modelling*** are central themes of our conference series and were also a central theme of this meeting. We use the term *multiscale* in an open and inclusive sense. There was much emphasis in presentations and discussions on

- Physics-based or/and data-driven
- Multiscale modelling
- Validation and accuracy
- Industry-academia similarities and differences in terms of barriers and conditions

Invited *keynote lectures* treated for example the booming area of machine-learned potentials, this approach is becoming an important tools to help overcome modelling barriers of time and space (Csányi). This is also the purpose of multiscale modelling – to cross the scales with models and workflows that reach more complex/realistic systems.

A *poster session* (with micropresentations), a *panel discussion*, and an appreciated *social exchanges* were also part of the program.

Keynote lectures

- **Gábor Csányi** (University of Cambridge, UK) "*First principles force fields*"
- **Ansgar Schäfer** (BASF, DE) *"Why BASF invests in atomistic modelling"*
- **Lilit Axner** (EuroCC National Competence Centers) *"Exascale computing, EuroCC and the HPC future"*
- **Erik Lindahl** (Stockholm Univ, SE) "*Strategies for spatial and temporal multiscale models of complex molecules with molecular dynamics*"
- **Stefaan Cottenier** (University of Ghent, BE) "*Testing the hell out of DFT codes with virtual oxides*"

Invited talks

- **Biplab Sanyal** (Physics, UU) *"DFT to tight-binding and beyond"*
- **Konstantin Neyman** (Physics, Univ of Barcelona) *"Ordering in bimetallic nanoparticles: Effects of environment"*
- **Bo Durbeej** (Chemistry, Linköping Univ) "*Multiscale Modelling in Photophysics: resolving a tricky fluorescence case in polar solution*"

Documentation

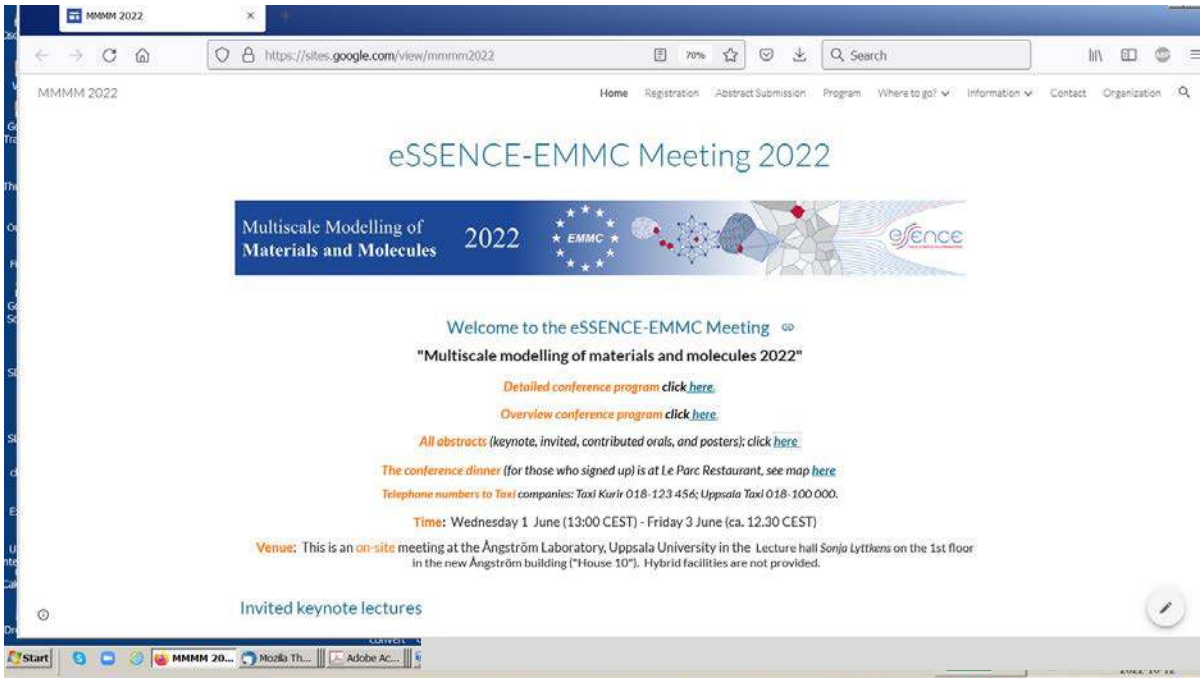
A 67-page booklet was produced with abstracts and program.

Selected recorded talks are currently being made available.

Photos were taken.

The website is still available.

From the conference website [(https://sites.google.com/view/mmmm2022)](https://sites.google.com/view/mmmm2022)



Transcript with links:

Detailed conference program* click *here.

Overview conference program* click *here.

All abstracts *(keynote, invited, contributed orals, and posters): click* ***here***

The conference dinner *(for those who signed up) is at Le Parc Restaurant, see map* ***here***

Telephone numbers to Taxi *companies: Taxi Kurir 018-123 456; Uppsala Taxi 018-100 000.*

Time: Wednesday 1 June (13:00 CEST) - Friday 3 June (ca. 12.30 CEST)

Venue: This is an on-site meeting at the Ångström Laboratory, Uppsala University in the Lecture hall *Sonja Lyttkens* on the 1st floor in the new Ångström building ("House 10"). Hybrid facilities are not provided.

Thank you to the EMMC !

The meeting organizers thank the EMMC for valuable support !

/ Kersti Hermansson (Uppsala University)