Multiscale Modelling Methods for Applications in Materials Science - CECAM - Tutorial 2013

	Monday 16 September	Tuesday 17 September	Wednesday 18 September	Thursday 19 September	Friday 20 September
9:00 – 10:30		*Thomas Frauenheim* **Atomistic Simulations Using the Approximate DFT Method DFTB+: Applications to Nanomaterials and Bio-Systems**	*Roland Faller* **Systematic Coarse Graining of Polymers and Biomolecules**	*Alejandro A. Franco* **Multiscale Modeling Methods for Electrochemical Energy Conversion and Storage**	*Martin Müser* **Modeling Charge Distributions and Dielectric Response Functions of Atomistic and Continuous Media Applications**
10:30 – 11:00		Coffee Break	Coffee Break	Coffee Break	Coffee Break
11:00 – 12:30	Registration	*Thierry Deutsch* **Introduction to Electronic Structure Calculations with BigDFT**	*Peter A. Bobbert* **Theory and Simulation of Charge Transport in Disordered Organic Semiconductors**	*Frank Ortmann* **Novel Electronics Materials: Large-Scale Charge Transport from First Principles**	*Jérôme Cornil* **Multiscale Modeling of Electronic Processes at Interfaces in Organic-Based Devices**
12:30 – 13:30	Lunch Break	Lunch Break	Lunch Break	Lunch Break	**Final Remarks** — Lunch Break
13:30 – 15:00	**Welcome** — *James A. Elliott* **Introduction to Multiscale Modelling of Materials**	**Visiting JSC Facilities** — *Thomas Frauenheim* *Ilian Todorov* **Practical Sessions**	*Michael Rambadt* **Introduction to UNICORE**	*Peter Råback* **Finite Element Modelling with Elmer**	Departure
15:00 – 16:00	Coffee Break		*Ivan Kondov / Stefan Bozic* *Thierry Deutsch* **Practical Sessions**	*Alejandro A. Franco* *Peter Råback* **Practical Sessions**	
16:00– 17:00	*Ilian Todorov* **Introduction to Modelling, Scalability and Workflows with DL_POLY**				
17:00– 17:30		**Poster Presentation**			
17:30 – 19:00	**Get-Together**	**Poster Session**			

Methods	
Applications	
Tools	
Hands-on	