

## Agenda

### Chemicals/Materials Track

- 8:30 Registration and Welcome Coffee
- 9:00 **Chairperson's Event Introduction:**  
Gerhard Engel, Senior Director R&D, Accelrys
- 9:15 **A Semi-empirical Molecular Orbital Study of Fullerene-encapsulated Mo-S/Mo-O Nanoclusters**  
James Elliott, Lecturer in Materials Modelling, University of Cambridge
- 9:45 **Finite Element Approaches to Mesoscopic Materials Modelling**  
Andrei Gusev, Researcher & Professor - Dept. of Materials MatSim GmbH & ETH Zurich
- 10:15 **Modelling Reactions at the Active Sites of Chiral Ruthenium Catalysts using Density Functional Theory**  
Sam French, Senior Scientist - Computational Chemistry Group, Johnson Matthey
- 10:45 Coffee Break
- 11:15 **Simulation of Atomic Scale Effects in Nano-CMOS Devices**  
Asen Asenov, Professor, Glasgow University
- 11:45 **Accelrys New Science: Future Developments in Materials Studio**  
Stephen Todd, Product Manager, Accelrys
- New Science in Contract Research Services: Case Studies, SIG's and Recent Initiatives**  
Patricia Gestoso-Souto, Senior Scientist, Accelrys
- 12:15 Lunch
- 13:45 **Versatile Biosensor Labels**  
Richard Gilbert, Principal Scientist, e2v Biosensors
- 14:15 **Hands-on Session: Materials Studio 4.2/Informatics**
- 16:00 Coffee Break
- 16:30 **Open Discussion and Q&As**
- 17:15 **Chairperson's Closing Remarks:**  
Gerhard Engel, Senior Director R&D, Accelrys

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