MEETING, JUNE 12, 2007
Agenda

8:00 - 9:15	**Registration**
9:15 - 9:30	Opening: **Jürgen Hafner** (University of Vienna) **Jakob Yngvason** (University of Vienna) Chair: **Erich Wimmer** (Materials Design)
9:30 – 10:00	**Ryoji Asahi** (Toyota Central R&D Labs., Inc.) • Materials design and development of functional materials for industry
10:00 – 10:30	**Joost van de Vondele** (University of Zurich) • Large scale simulations with CP2K: investigating electron transfer at a solid/liquid interface
10:30 – 11:00	**Chris Wolverton** (Ford and Northwestern) • Discovery of novel hydrogen storage materials: An atomic scale computational approach
11:00 – 11:30	**Martijn Marsman** (University of Vienna) • Hybrid functionals applied to extended systems
11:30 – 12:00	**Christophe Domain** (EDF) • Density functional calculations on structural materials for nuclear energy and functional materials for photovoltaic energy
12:00 – 13:30	**Lunch break**
	Chair: **Chris Wolverton** (Northwestern University)
13:30 – 14:00	**Richard Needs** (University of Cambridge) • Quantum Monte Carlo - electron correlation from random numbers
14:00 – 14:30	**Susanne Opalka** (United Technologies) • Design of water gas shift catalysts for H_2 production in membrane reactors
14:30 – 15:00	**Chris van der Walle** (University of Santa Barbara) • Controlling the conductivity of wide gap-semiconductors (nitrides and oxides)
15:00 - 15:30	**Coffee break**
15:30 - 16:00	**Don Siegel** (Ford Motor) • First-principles computation as a guide to the design of new hydrogen storage materials
16:00 – 16:30	**Artem Oganov** (ETH Zurich) • Evolutionary crystal structure prediction: a novel approach to materials design
16:30 – 17:00	**Wolfgang Mannstadt** (Schott AG) • Computational material science aided design of glass ceramics and crystal properties
17:00 – 17:30	**Tomas Bucko** (University of Vienna) • Ab-initio calculations of free-energy reaction barriers
17:30	**Posters and Reception**

MEETING, JUNE 13, 2007
Agenda

Chair: **Ryoji Asahi** (Toyota Research)

9:00 - 9:30 **Emilio Artacho** (University of Cambridge)
- Gearing for complexity: Recent developments around linear-scaling materials calculations and the SIESTA program

9:30 - 10:00 **Pascal Raybaud** (Institut Français du Pétrole)
- Industrial supported catalysts in working states: DFT insights beyond all expectations

10:00 – 10:30 **Jutta Rogal** (FHI Berlin)
- Catalytic oxidation at surfaces: Insight from first-principles statistical mechanics

10:30 – 11:00 **Coffee break**

11:00 – 11:30 **Betty Coussens** (DSM Research Laboratories)
- A systematic computational study of electronic effects on hydrogen sensitivity of olefin polymerisation catalysts

11:30 – 12:00 **Georg Kresse** (University of Vienna)
- Accurate band gaps and dielectric properties from one electron theories

12:00 – 12:30 **Berit Hinneman** (Topsoe)
- Theoretical and experimental studies of MoS_2, CoMoS and NiMoS hydrotreating catalysts

12:30 – 14:00 **Lunch break**

Chair: **Georg Kresse** (University of Vienna)

14:00 – 14:30 **Fumiyasu Oba** (University of Kyoto)
- First principles calculations for ceramic science and engineering

14:30 – 15:00 **Petrie Steynberg** (Sasol Technologies)
- DFT bulk and selected surface analysis of Hagg Fe-Carbide (Fe5C2)

15:00 – 15:30 **Matthieu Verstraete** (University of York)
- First-principles computation of the electronic and dynamical properties of solids and nanostructures with ABINIT

15:30 – 16:00 **Coffee break**

16:00 – 16:30 **Kurt Stokbro** (Atomistix)
- First principles modeling of electron transport across interfaces

16:30 – 17:00 **Lars Nordström** (Uppsala University)
- Calculation of technologically important aspects of magnetism: Anisotropy, critical temperatures and spin dependent transport

17:00 - 17:30 **Oleg N. Mryasov** (Seagate)
- Multiscale modeling of nanophase materials and devices for magnetic recording

MEETING, JUNE 14, 2007
Agenda

Chair: **Richard Needs** (University of Cambridge)

9:00 - 9:30 **Clint Geller** (Bechtel-Bettis)
- Electronic structure modeling in an engineering context

9:30 - 10:00 **Chris Skylaris** (University of Southhampton)
- The ONETEP program for linear-scaling density functional calculations with plane waves: applications and recent developments

10:00 – 10:30 **Sadasivan Shankar** (Intel)
- Density functional theory and beyond: Opportunities for quantum methods in materials modeling for semiconductor technology

10:30 – 11:00 **Coffe break**

11:00 – 11:30 **Thomas Bligaard** (TU Lyngby)
- Computational alloy catalyst design

11:30 – 12:00 **Louis Hector** (General Motors)
- Ab initio simulations of hydrogen storage materials at General Motors R&D Center: An overview of light and heavy metal hydride property predictions

12:00 – 12:30 **Karsten Held** (MPI Stuttgart)
- Band structure meets many-body theory: the LDA+DMFT method

12:30 – 14:00 **Lunch break**

Chair: **Raimund Podloucky** (University of Vienna)

14:00 – 14:30 **Robert Laskowski** (Vienna University of Technology)
- Unraveling the structure of the BN/Rh(111) nanomesh with ab-initio calculations

14:30 – 15:00 **Hansong Cheng** (Air Products)
- A mechanistic study on hydrogen spillover onto carbon based materials

15:00 – 15:30 **Rajeev Ahuja** (Uppsala University)
- Materials Design from ab initio Calculations: Nanolayered MAX phases

15:30 – 16:00 **Coffee break**

16:00 – 16:30 **Miguel Gosalvez** (University Nagoya)
- VisualTAPAS: an example of DFT-assisted understanding and simulation of anisotropic etching

16:30 – 17:00 **Yasunari Zempo** (Sumitomo Chemical)
- Practical application of computational materials science in the development of optical materials

17:00 **Closing**