

The 3rd *Theory Meets Industry* International Workshop  
(TMI 2009) Program

**Wednesday, November 11, 2009**

9:30	Opening
Session 1	Chair: Erich Wimmer
9:50 – 10:30	<b>Jürgen Hafner</b> ( <i>University of Vienna, Austria</i> ) Ab-initio density-functional calculations in materials science: From spintronics to catalysis
10:30 – 11:10	<b>Christophe Domain</b> ( <i>EDF, France</i> ) Density functional calculations of material properties for energy production
11:10 – 11:50	<b>Ryoji Asahi</b> ( <i>Toyota Central R&amp;D Labs, Japan</i> ) The role of first-principles calculations in development of functional materials for energy harvesting
11:50 – 13:30	<i>Lunch and Coffee</i>
Session 2	Chair: Christophe Domain
13:30 – 14:10	<b>Takeo Fujiwara</b> ( <i>The University of Tokyo, Japan</i> ) Large-scale electronic structure calculation theory and applications
14:10 – 14:50	<b>Gábor Csányi</b> ( <i>University of Cambridge, UK</i> ) Gaussian approximation potentials: the accuracy of quantum mechanics, without the electrons
14:50 – 15:10	<i>Coffee</i>
Session 3	Chair: Takeo Fujiwara
15:10 – 15:50	<b>Stefan Müller</b> ( <i>University of Erlangen-Nuremberg, Germany</i> ) First-principles based modelling of alloys
15:50 – 16:30	<b>Isao Tanaka</b> ( <i>Kyoto University, Japan</i> ) Phase relationships and structures of inorganic crystals by combination of cluster expansion method and first principles calculations
16:30 – 16:50	<i>Coffee</i>
Session 4	Chair: Tomoyuki Yamamoto
16:50 – 18:10	Poster Preview (2 min. each)
19:00 – 21:00	<i>Banquet</i>

**Thursday, November 12, 2009**

Session 5	Chair: Tamio Oguchi
9:00 – 9:40	<b>Bernard Delley (Paul Scherrer Institute, Switzerland)</b> DFT studies from molecules to surfaces, solids and liquids with DMol <sup>3</sup>
9:40 – 10:20	<b>Shinichiro Nakamura (Mitsubishi Chemical, Japan)</b> Theoretical chemistry in chemical industrial research, NMR- $\delta$ for large proteins via FMO method
10:20 – 10:40	<i>Coffee</i>
Session 6	Chair: Bernard Delley
10:40 – 11:20	<b>Werner Janse van Rensburg (Sasol Technology, South Africa)</b> A DFT investigation of fundamental aspects of the Fischer-Tropsch mechanism on iron carbide surfaces
11:20 – 12:00	<b>Katsuyuki Matsunaga (Kyoto University, Japan)</b> Theoretical pH dependent defect energetics in calcium phosphate bioceramics
12:00 – 13:40	<i>Lunch and Coffee</i>
Session 7	Chair: Shinichiro Nakamura
13:40 – 14:20	<b>Pascal Raybaud (IFP, France)</b> Rational exploration of optimal chemical properties: From bulk storage materials to catalytic amorphous surfaces
14:20 – 15:00	<b>Tomas Bucko (University of Vienna, Austria)</b> Role of entropy in catalytic reactions - Application to hydrocarbon transformations
15:00 – 15:20	<i>Coffee</i>
Session 8	Chair: Pascal Raybaud
15:20 – 16:00	<b>Georg Kresse (University of Vienna, Austria)</b> The random phase approximation (RPA) to correlation: Quasiparticles and total energies
16:00 – 16:40	<b>Takao Kotani (Tottori University, Japan)</b> Quasiparticle self-consistent GW method applied to transition metal oxides
Poster Session	Chair: Hiroki Moriwake
16:40 – 18:30	Poster session

## Friday, November 13, 2009

Session 9	Chair: Masato Yoshiya
9:00 – 9:40	<b>Masaya Ishida</b> ( <i>Sumitomo Chemical, Japan</i> ) Practical application of computational materials science for industrial inorganic materials
9:40 – 10:20	<b>George Fitzgerald</b> ( <i>Accelrys, USA</i> ) A high-throughput computational approach for materials design and optimization
10:20 – 10:40	<i>Coffee</i>
Session 10	Chair: Göran Wahnström
10:40 – 11:20	<b>Tamio Oguchi</b> ( <i>Hiroshima University, Japan</i> ) Surface Rashba effect: Spin-orbit coupling and symmetry
11:20 – 12:00	<b>Alessandro De Vita</b> ( <i>King's College London, UK</i> ) Modelling the chemo-mechanics of brittle fracture: A fundamental problem and a case for industrial partnerships
12:00 – 13:40	<i>Lunch and Coffee</i>
Session 11	Chair: Alessandro De Vita
13:40 – 14:20	<b>Masanori Kohyama</b> ( <i>AIST, Japan</i> ) First-principles analysis and design of materials interfaces
14:20 – 15:00	<b>Göran Wahnström</b> ( <i>Chalmers University of Technology, Sweden</i> ) Theory of metal-ceramic interfaces
15:00 – 15:20	<i>Coffee</i>
Session 12	Chair: Masanori Kohyama
15:20 – 16:00	<b>Fumiyasu Oba</b> ( <i>Kyoto University, Japan</i> ) Point defects in oxide semiconductors: An approach from first principles
16:00 – 16:40	<b>Erich Wimmer</b> ( <i>Materials Design, USA</i> ) Ab initio calculations for industrial materials engineering: Successes and challenges
16:40 – 16:50	Closing remarks