

## FIRST EUROMINSCI CONFERENCE

26-29 March 2007, *La Colle-sur-Loup (near Nice), France*

### CONFERENCE PROGRAMME

last update: 22 March 2007

#### Monday 26 March 2007

- 12.00-13.30 Lunch and Registration at the ESF desk
- 13.30-14.00 **Conference Opening**  
Bernard Avril (EUROCORES Programme Coordinator, ESF) & Björn Winkler  
(Chair of the EuroMinSci Scientific Committee)

#### Session 1: Mineral Physics and Geosciences Chair: Björn Winkler

14.00 **Robert Liebermann** (COMPRES, Stony Brook, US)  
*Outdoor vs indoor geophysics*

15.00-15.30 **Discussion**

15.30 Coffee break

#### Session 2: Linking Experimental and Computational Mineral Physics Chair: Leonid Dubrovinsky

16.00 **Sandro Scandolo** (ICTP, Trieste, IT)  
*Quantum simulations as a window into the interior of the Earth*

16.45 **Björn Winkler** (Johann Wolfgang Goethe Universität, Frankfurt, DE)  
*Structure and properties of hydrous minerals from experiment and computation*

17.05-17.15 **Discussion**

**Session 3: Introduction to the CRPs – Part I**  
Chair: Bernard Avril

- 17.15      **Thierry Alboussière** (Université Joseph-Fourier, Grenoble, FR)  
*GRICO - Growth of the Inner Core: Structure and Dynamics*
- 17.30      **Nora De Leeuw** (University College London, UK), representing **Laurent Charlet**  
*CUBCAT - Reactivity of (Fe,Ni)S minerals and cubane clusters with gas and amino-acids: towards an understanding of the emergence of life*
- 17.45      **Richard Harrison** (University of Cambridge, UK)  
*MICROMAGN - Magnetism and microstructure: from the nanometre to the planetary scale*
- 18.00      **David Dobson** (University College London, UK)  
*EuroSLAB - The rheology of the subducting slab and mantle*
- 18.15      **Leonid Dubrovinsky** (Universität Bayreuth, DE)  
*MCEC - Mineralogy and Chemistry of Earth's core*
- 18.30      **Sandra Piazzolo** (Stockholm University, SE)  
*MINSUBSTRDYN - Subgrain structure development in rocks and metals*
- 18.45      Welcome gathering
- 19.30      Dinner
- 21.00      Informal poster session

**Tuesday 27 March 2007**

**Session 4: Mineral Physics of the Earth's Mantle & Core – Part I**  
Chair: David Dobson

- 09.00      **Hans Keppler** (Universität Bayreuth, DE)  
*The origin of Earth's asthenosphere*
- 09.45      **Wilson Crichton** (ESRF, Grenoble, FR)  
*Illumination of the Earth's deep interior by synchrotron radiation*
- 10.30      Coffee break

**Session 5: Mineral Physics of the Earth's Mantle & Core – Part II**  
Chair: David Dobson

- 11.00      **David Mao** (Carnegie Institution of Washington, US)  
*New opportunities in experimental mineral physics of mantle and core*
- 12.00      **James Wookey** (University of Bristol, UK)  
*Constraints from seismic anisotropy on the mineralogy the lowermost mantle*

- 12.20 **David Mainprice** (Université de Montpellier II, FR)  
*Mineral elasticity to seismic anisotropy in subduction zones*
- 12.40 Lunch

**Session 6: Microstructure and Mineral Behaviour – Part I**  
Chair: Martin Dove

- 14.00 **Paul Bons** (Eberhard Karls University, Tübingen, DE)  
*Numerical modelling of substructure dynamics with Elle*
- 14.30 **Andréa Tommasi** (Université de Montpellier II, FR)  
*Multiscale modeling of deformation and anisotropy in the mantle*
- 14.50 **Richard Harrison** (University of Cambridge, UK)  
*Magnetism and microstructure: from the nanometre to the planetary scale*
- 15.20 **Discussion**
- 15.30 Coffee break

**Session 7: Microstructure and Mineral Behaviour – Part II**  
Chair: Sandra Piazzolo

- 16.00 **Suzanne McEnroe** (Geological Survey of Norway, Trondheim, NO)  
*Magnetic properties of oxides from a large remanence-dominated magnetic anomaly in south Australia: importance of intergrowths and implications for planetary magnetization*
- 16.20 **Alberto Perez-Huerta** (University of Glasgow, UK)  
*Mg distribution and crystallography in two different calcite organisms: how reliable is Mg:Ca as a temperature proxy?*
- 16.40 **Daniel Tatham** (University of Liverpool, UK)  
*In situ heating and deformation experiments in the SEM*
- 17.00 **Discussion**
- 17.10 Coffee break

**Session 8: Introduction to the CRPs – Part II**  
Chair: Bernard Avril

- 17.40 **Jean-Pierre Cuif** (Université de Paris XI, FR)  
*BioCalc - Calcareous Biocrystals*
- 17.55 **Alberto Garcia** (CSIC, Barcelona, ES)  
*ORION - Ordering of Ions in Minerals*
- 18.10 **Björn Winkler** (Johann Wolfgang Goethe Universität, Frankfurt, DE)

*HydroMin - Hydrogen in Minerals*

**Session 9: New views on the Asthenosphere and the Transition Zone**  
Chair: Jean-Pierre Cuif

- 18.25-19.10     **David Dobson** (University College London, UK)  
*The origin of Deep Seismicity*
- 19.30             Dinner
- 21.00             **Informal poster session**

**Wednesday 28 March 2007**

**Session 10: Atomistic Understanding of Minerals**  
Chair: Alberto Garcia

- 09.00             **Eduardo Hernández** (CSIC, Barcelona, ES)  
*Obtaining phase coexistence conditions and phase diagrams from atomistic simulations: techniques and sample applications*
- 09.45             **Etienne Balan** (Université Paris VI, FR)  
*Nature and properties of OH stretching modes in hydrous minerals: new insights from first-principles calculation*
- 10.10             **Michael Fetchelkord** (Ruhr-Universität Bochum, DE)  
*Ordering of F/OH anions as a function of the Al/Mg cation distribution in the octahedral sheets of phlogopite studied by Solid State NMR spectroscopy*
- 10.30             Coffee break

**Session 11: Elements and Alloys at Extreme Conditions**  
Chair: Thierry Alboussière

- 11.00             **Igor Abrikosov** (Linköping University, SE)  
*First-principles simulations of alloy thermodynamics in megabar pressure range*
- 11.20             **Leonid Dubrovinsky** (Universität Bayreuth, DE)  
*Iron-nickel alloy at conditions of deep Earth interiors*
- 11.40             **Sergei Simak** (Linköping University, SE)  
*First-principles theory of elements under high pressure*
- 12.00             **Rajeev Ahuja** (University of Uppsala, SE)  
*Structural and electronic behaviors of iron dissolving in MgSiO<sub>3</sub> Perovskites from first-principles theory*
- 12.20             **Arkady Mikhaylushkin** (Uppsala University, SE)

*Iron at extremely high pressure and temperature conditions*

12.30 Lunch

**Session 12: Reactivity & Structure of Surfaces & Interfaces – Part I**  
Chair: Nora de Leeuw

- 14.00 **Andrew Putnis** (Westfälische Wilhelms Universität Münster, DE)  
*Interface-coupled dissolution-reprecipitation as a general mechanism of reequilibration of minerals in contact with a fluid phase*
- 15.00 **Tony Devey** (University College London, UK)  
*The computational determination of the structure, magnetic properties and elastic constants of mackinawite using ab-initio methods*
- 15.15 **Gernot Nehrke** (Alfred-Wegener Institut für Polar- und Meeresforschung, Bremerhaven, DE)  
*Calcite growth rate and solution stoichiometry, implications for biomineralization*
- 15.30 Coffee break

**Session 13: Reactivity & Structure of Surfaces & Interfaces – Part II**  
Chair: John Tse

- 16.00 **Margaret Cusack** (University of Glasgow, UK)  
*Magnesium and sulphur (Micro-XANES mapping) in the shell of the brachiopod *Terebratulina retusa**
- 16.20 **Yannicke Dauphin** (Université de Paris XI, FR)  
*Biochemical characterizations of the organic matrices of coral skeletons and mollusc shells*
- 16.40 **Jean-Pierre Cuif** (Université de Paris XI, FR)  
*Microstructural patterns of nucleation and growth in the crystal-like calcitic prisms of the Bivalve shells*
- 17.10 **Wolfgang Moritz** (Universität München, DE)  
*The structure of the hematite (0001) surface investigated by LEED*

**Session 14: Official Poster Presentation**

- 17.30-19.30 **Official Poster Presentation**  
*Each principal poster author should be in attendance*
- 20.00 **Conference dinner** and presentation of best poster awards

Thursday 29 March 2007

**Session 15: Defects and Disorder in Materials**  
Chair: Alberto Garcia

- 09.00           **Martin Dove** (University of Cambridge, UK)  
*Dynamics of silicate networks*
- 09.45           **Denis Machon** (Université Lyon 1, CNRS, FR)  
*Pressure-induced amorphization: the ferroelastic glass concept*
- 10.15           **John Tse** (University of Saskatchewan, CA)  
*Computational high pressure science*
- 11.00           Coffee break

**Session 16: General Discussion about EuroMinSci & Future Opportunities**  
Chair: Björn Winkler

- 11.30           **Volker Heine** (Cambridge University, UK)  
*Summary remarks*
- 12.00-12.30   **Conclusive discussions**
- 12.30           Lunch and departure

**All posters will be on display during the whole duration of the conference**

*EuroMinSci is financed by research agencies from 12 European countries: Austria (FWF), Belgium (FWO, FNRS), Czech Republic (CSF), Estonia (ETF), France (CNRS), Germany (DFG), Hungary (MTA), Italy (CNR), Slovakia (SAV), Spain (MEC), Sweden (VR), United Kingdom (NERC), and the European Science Foundation (ESF) under the EUROCORES Programmes through support by the European Commission, DG Research (Sixth Framework Programme, contract ERAS-CT-2003-980409).*