

## **THEORETICAL AND COMPUTATIONAL METHODS IN MINERAL PHYSICS: APPLICATIONS TO GEOPHYSICS**

**Dates:** Short Course sessions are Friday and Saturday, December 11-12, 2009 (preceding the Annual fall meeting of the American Geophysical Union in San Francisco). There is a reception for participants starting at 6 pm Thursday evening, December 10. The Short Course will start at 8:15 am on Friday, December 11, and end 7 pm the evening of Saturday, December 12. Departure is on Sunday December 13 after breakfast.

**Location:** Short Course sessions are at the Doubletree Hotel & Executive Meeting Center Berkeley Marina, 200 Marina Blvd., Berkeley, CA 94710, United States, Tel: +1 (510) 548-7920.

**Convenors:** *Renata Wentzcovitch:* University of Minnesota, Dept of Chemical Engineering & Materials Science, 421 Washington Ave SE Ste 151, Minneapolis MN 55455-0132, USA; Tel: +1 (612) 625-6345; wentzcov@cems.umn.edu.

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<b>Fees:</b>		<i>on or before 10/31/2009</i>	<i>after 10/31/2009</i>
Professional Registration:	Member ‡	\$350	\$400
	Non-member	\$445*	\$495*
Student Registration:	Member ‡	\$100	\$150
	Non-member	\$140*	\$190*
Speaker		no cost	no cost

‡ Mineralogical Society of America (MSA) and Geochemical Society (GS) members.

\*includes 2010 MSA membership dues and electronic access to *American Mineralogist*.

**Registering:** Online registration is at <http://www.minsocam.org/MSA/SC/#TACM>. Printable registration forms are also available online, and from the MSA Business Office, 3635 Concorde Pkwy Suite 500, Chantilly, VA 20151-1110 USA. phone: +1 (703) 652-9950; fax: +1 (703) 652-9951; e-mail: jaspeer@minsocam.org. Registration forms with payment must be returned to the MSA Business Office. Registration fees will be partially refunded if cancellation is received in writing on or before November 1, 2009. All participants and speakers must register.

**Practical:** Registration fee includes MSA/GS short course sessions, the *Reviews in Mineralogy and Geochemistry* volume, Thursday evening reception, continental breakfast Friday, Saturday and Sunday, mid-morning and mid-afternoon refreshments and lunch on Friday and Saturday, and dinner on Friday. Registration fee does not include room, other meals, or any transportation costs to or from the short course site. Both participants and speakers must make arrangements and pay their own lodging and transportation. Participants need to contact the Doubletree Hotel & Executive Meeting Center Berkeley Marina, 200 Marina Blvd., Berkeley, CA, United States 94710, Tel: +1 (510) 548-7920 or +1 (800) 243-0625 to make reservations and pay for your lodging. (The room reservation code is MSA or MSA Computational Methods Short Course).

**Short Course description:** The objective of this course is to review the important techniques used in theoretical and/or computational mineral physics today, along with exemplary applications that have contributed to advance the field of high pressure mineral physics and geophysics. It is time for publication of a comprehensive overview of the state of this field that has matured and several approaches that have flourished within the last fifteen years are here to stay.

The emphasis of the course is on geophysics and condensed phases. The methods and applications that will be discussed were developed primarily in the condensed matter and solid state physics communities. The focus will be high pressure, high temperature bulk properties, such as thermoelastic and thermodynamics properties in single and multiphase aggregates. The outcome of these studies is geared towards understanding planetary interiors, interpretation of seismic observations, and providing essential constraints for geodynamic simulations.

The computational approaches introduced in this course have contributed to the establishment of a field of research that today rivals experimental methods: they are predictive. Their applications are increasing at very rapid pace now, and the future of this research field is bright. Experimentalists, seismologists, and geodynamicists should be aware of these methods and results they can produce. Students should be inspired by the possibilities presented by this collection of articles. The issue will likely be well received by the materials physics, materials sciences, and simulations communities as well since mineral physics presents challenges not always faced by these other fields. Mineral physics explores properties of condensed systems in a wider range of pressures and temperatures. The experiences of those active in mineral physics are invaluable and should be communicated to researchers active in related fields.

### Short Course Topics and chapter titles for RiMG Volume

- Review of exchange correlation treatments in density functional based calculations..... John Perdew (Tulane University, Physics Department)
- Density Functional Perturbation Theory and applications to phonons.....Stefano Baroni (International School for Advanced Studies, Trieste, Italy)
- Quasiharmonic theory of elastic properties .....Renata Wentzcovitch (Department of Chemical Engineering and Materials Sciences, U. of Minnesota)
- Quantum Monte Carlo methods for electronic structure calculations .....David Ceperley (University of Illinois at UrbanaChampaign, Physics Department)
- Application of QMC Methods in mineral physics ..... Ron Cohen (Carnegie Institution of Washington)
- Theoretical studies of diffusion in Earth materials ..... John Brodholt (Department of Earth and Planetary Sciences, UCL, London)
- Plasticity in Earth materials.....Patrick Cordier (Laboratoire de Structure et Proprietes de l'Etat Solide, CNRS/Universite de Lille 1)
- Thermal conductivity of Earth materials ..... Stephen Stackhouse, (Department of Geological Sciences, University of Michigan)
- Structural predictions with genetic algorithms..... Artem Oganov (Department of Geosciences, Stony Brook University)
- Multimegabar mineralogy .....Koichiro Umemoto (Department of Geology and Geophysics, University of Minnesota)
- Iron at core conditions .....Dario Alfe (Department of Physics, UCL, London)
- Silicate and oxide melts ..... Bijay B. Karki (Department of Computer Science, Louisiana State University)
- Planetary fluids..... Burkhard Militzer (Department of Earth and Planetary Sciences, UC Berkeley)
- Advances in the DFT+U method for strongly correlated materials.....Matteo Cococcioni (Department of Chemical Engineering and Materials Sciences, U. of Minnesota)
- Spin transitions in mantle minerals.....Renata Wentzcovitch (Department of Chemical Engineering and Materials Sciences, U. of Minnesota)
- Cluster expansion methods in Earth materials ..... Victor Vinograd (Goethe University, Germany)
- First principles spectroscopy of hydrous and nominally anhydrous minerals .....Keith Refson (Rutherford Appleton Laboratory, UK)
- Interatomic potentials in mineral physics .....Julian Gale (Western Australian Nanochemistry Research Institute, Australia)
- Large Scale simulations in mineral physics ..... Mark Ghiorso (OFM Research)
- Thermodynamics of multi-phase aggregates..... Lars Stixrude (UCLLondon, UK)

**Student Support:** Students are eligible for \$600 in scholarship. Simply register as a “Student member or non-member” and e-mail to Debbie Schutta (dschutta@msi.umn.edu) a letter from your advisor stating the stage of your research and expected degree date. Post-docs will also be considered depending on the number of student registrations. A similar letter must be sent.

**Meeting Session:** The short course will be held in conjunction with an AGU-sponsored topical session at the subsequent annual fall AGU meeting, “*MR05 Computational Approaches and Applications in Mineral Physics*“. If you submit an abstract for this session, please inform the convenors.