RENATA M. M. WENTZCOVITCH, Prof. of Materials Science and Engineering
http://research.cems.umn.edu/wentzcovitch/

Professional Preparation

University of São Paulo	Physics	B.A., *1980*
University of São Paulo	Physics (with Prof. José R. Leite)	M.Sc., *1982*
UC Berkeley	Physics (with Prof. Marvin L. Cohen)	Ph.D., *1988*

Appointments

- Prof. in Chemical Engineering and Materials Science, UMN, *2006-present*
- Assoc. Prof. in Chemical Engineering and Materials Science, UMN, *2001-06*
- Member of UMN Graduate Faculty in School of Physics and Astronomy, Department of Earth Sciences, Scientific Computation Program, Chemical Physics Program, *2004-present*
- Asst. Prof. in Chemical Engineering and Materials Science, UMN, *1994-2001*
- Post-doc, Physics, Stony Brook Univ. and Brookhaven, with Prof. Philip B. Allen, *1989-1992*
- Post-doc, Physics, Cavendish Labs, Cambridge, and Royal Institution of Great Britain, *1992-94*

Honors and Awards

Wilhelm Heraeus Visiting Prof.ship, Goethe University at Frankfurt am Main (*2015-16*) • Fellow, AAAS (*2013*-) • Fellow, AAAS (Physics) (*2012*-) • Fellow, MSA (*2009*-) • Fellow, AGU (*2008*-) • Fellow, APS, Materials Physics (*2006*-) • Alexander von Humboldt Award for US-Scientists (*2008*) • JSPS, Invitation Fellowship for Research in Japan (*2008*) • Member at-large, APS, Comp. Physics (*2000-03*) • Fellow (*2001*-) and Assoc. Fellow (*1997-2001*) of Minnesota Supercomputing Inst. • "Graduate Research Award" of the MRP Group, AGU (*2009*), PhD thesis of Y. Yu • "Outstanding Student Paper Award" of the MRP Group, AGU (*2009*) to M. Núnez-Valdez • Shell Land-Grant Prof. in Chemical Engineering and Material Science, UMN (*1994-1995*) • Honorary Research Fellow, University of London (*1993-1994*) • Fellowships from Brazilian agencies: FAPESP (undergraduate, *1978-1980*), CNEN (graduate, *1980-82*), CNPq (*1983-87*)

Synergistic Activities

At other institutions: Assoc. Investigator at ELSI, WPRI of the JSPS, Tokyo Tech (*10/12*-) • Visiting Prof., Computational Science Research Center, Chinese Academy of Engineering Physics (*06/15*) • Visiting Prof., Department of Earth and Space Sciences, University of Science and Technology of China, (*07/12, 8/13*) • Visiting Prof., Faculty of Sciences, Interactive Center for Science, Tokyo Tech (*5/10-8/10*) • Visiting Prof., Departments of Physics and Earth and Planetary Sciences, Tokyo Tech (*04/02, 08/06, 10-12/08*) • Visiting Prof., Departments of Geology, University of Frankfurt (*09/08-11/08, 08/09, 08/10, 08/12*) • Visiting Prof. Department of Physics and Astronomy and Department of Geological Sciences, (*Fall'05*) and Department of Physics and Astronomy (*08/95, 02/96, 08/97, 07/98*), Stony Brook University • Distinguished Visiting Prof. (*2005*), Visiting Prof. (*08/01, 08/02, 08/03, 08/04, 08/12*) and Visiting Scientist (*08/98, 08/99, 08/00*), SISSA • Visiting Scientist, INESC, Lisbon (*01/96*) • Asst. Prof., Department of Materials Physics, Institute of Physics, U of São Paulo, Brazil (*Fall'95*)

Other professional activities: Director of Graduate Studies, Scientific Computing Program, UMN (*2012*-) • Founding Director, Virtual Laboratory for Earth and Planetary Materials, *VLab,* Minnesota Supercomputing Institute, UMN (*2004-10*) • Assoc. Editor, *American Mineralogist*, (*2011*-) • UMN representative and elector to the NSF-COMPRES consortium (*2003*-) • UMN Point-of-Contact for the UMN/Tokyo Tech Cooperation in Graduate Program (*2013*-) • Referee for APS, ACS, MRS, AGU, AAAS, UK, and EU-based journals • Regular referee for US (NSF, DOE, PRF), UK (SERC and NERC), German (DGF), and Italian (MIUR) funding agencies.

Committee Services

Aneesur Rahman Prize APS/DCOMP, vice-chair (*2012*), chair (*2017*) • APS Fellow Nominating (*2008-11)* • Bridgman Award Selection, AIRAPT (*2009-11*) • Status of Women in Physics (site visit team member to U. Washington (*2005*) • APS March Meeting Program *(2002-03)* • *COMPRES*, Long range planning and co-author of NSF report: *"Understanding the Building Blocks of our Planet: The Materials Science of Earth Processes"* (*2010*).

At U of M**:** Grad recruiting, CEMS (*1994, 2005-6, 2011-12*) • Faculty recruiting, CEMS (*2005-06*) and Earth Sciences (*2013*) • Nominating, MSI (*1997-99,2001-03*) • MSI/IBM-SP Advisory (*1997-98*) • MSI Research Scholarship (*2003-06,* Chair in *2006*) • DTC/MSI Task Force on Initiatives in High Performance Computing (*2006-07*) • MSI Long-range Planning (*2006-07*) • MSI Allocation (*2009-12*), Chair (*2010*) • OVPR Grant-in-Aid for Research and Scholarship review (*2013*) • Basic Sciences Computing Lab Steering (*2000-01*) • CSE Instructional Computing (*1999-00*) • President's Distinguished Faculty Mentor Program (*1998-2001*).

Panels

Review of DOE-EFRC, High Pressure Energy Research in Extreme Environments, Carnegie Institution of Washington, Geophysical Lab (*2012*) • Review of DOE-EFRC, Center for Emerging Superconductivity, BNL/ANL/UIUC (*2012*) • Review of DOE Theoretical Chemical Physics Program at PNL (*2010*) • NSF: XSEDE's 2nd Annual review panel (*2013*) • NSF: Review panel for OCI/SI2 Software Institutes (*2012*) • NSF: High Performance Computing (track 2b) (*2006,2009*) • NSF: Materials World Network: Cooperative Activity in Materials Research between US Investigators and Counterparts Abroad (MWN) (*2007*) • Joint NSF-DFG Materials Research Review Panel, Berlin (*2007*) • NSF: ASU MRSEC (*1999*).

Workshop/Conference/Mimi-Course organization

Lead organizer (w/A. Navrotsky), 2016 COMPRES Meeting Breakout Session "Infrastructure for Computational/Theoretical Mineral Physics" • Lead organizer (w/L. Arrachea (AR), E. Miranda (BR), and R. Martin (USA)), Workshop: *Next Generation Quantum Materials*, (ICTP-SAIFR), São Paulo, Brazil (*04/16*) • Instructor of Mini-Course: *Ab Initio Modeling of Materials at Extreme Conditions,* Materials Physics, U. São Paulo (*05/15*) • Organizer: Computational Approaches in High Pressure Research, High Pressure Workshop of the IUC, Campinas, Brazil (*09/15*) • Lead organizer, co-organizer D. Bercovici, Symposium: *Modeling Earth's Interior from Atomic to Global Scale*, AAAS Annual Meeting *(02/15)* • Instructor of Mini-Course: *Ab Initio Modeling of Materials at Extreme Conditions,* Materials Physics, U. São Paulo (*05/15*) • Lecturer and instructor of computational labs for the *African School of Electronic Structure Methods and Applications* **(ASESMA)** (two week program): African Institute for Mathematical Sciences*,* Cape Town (*07/10*); Chepkoilel College*,* Eldoret, Kenya (*05/12*) • Co-organizer, MRP Sessions, *The role of transition elements in geophysical and geochemical processes in the deep Earth*, Fall **AGU** Meeting (*12/14*) • Co-organizer, MRP Sessions, *Thermodynamic & Elasticity Databases and the Geoinformatics Revolution: Objectives, Scope and Construction of Data Systems for Geochemical and Geophysical Modeling*, Fall **AGU** Meeting (*12/13*) • Co-organizer, MRP Sessions, *Electronic and Elastic properties of Mantle Materials*, Fall **AGU** Meeting (*12/12*) • Lead-organizer, co-organizer D. Truhlar, Symposium: *Quantum chemistry meets geochemistry*, **ACS** National Meeting (*03/12*) • Co-organizer, MRP Sessions, *Deep Mantle Properties*, Fall **AGU** Meeting (*12/10*) • Co-organizer, MRP Physics Sessions, *Recent Advances in Understanding Dynamics, Structure, and Composition of the Deep Lower Mantle*, Joint Assembly, Spring **AGU** Meeting (*05/09*) • Co-organizer, MRP Sessions, *Spin Crossover Transitions in the Lower Mantle*, Fall **AGU** Meeting (*12/08*) • Co-organizer, MRP Sessions,

Computational Mineral Physics, Spring **AGU** Meeting *(05/06, 12/07, 12/08, 12/09)* • Co-organizer, MRP Sessions, *Post-perovskite Phase Transition and the D" Layer*, Fall **AGU** Meeting *(12/04)* • Co-organizer: Focus Session *Computational Chemistry for Geochemistry*, 243rd ACS National Meeting (*03/12*) • Organizer*, "Infrastructure for Computational Mineral Physics: a Community Consultation Workshop"*, for NSF's **COMPRES** (*08/10*). Co-author of *"Infrastructure for Computational Mineral Physics: a Community Consultation Workshop"* report to COMPRES • Co-organizer: Workshop on *Computational Mineral Physics: Geophysical Applications* at the Centre Européen de Calcul Atomique et Moléculaire (**CECAM**), with Hans-Peter Bunge and Lappo Boschi, ETH Zurich (*10/10*) • Organizer "*Theoretical and Computational Methods in Mineral Physics: Geophysical Applications*", Joint Short Course for the Mineralogical Society of America and ***VLab***, Berkeley CA, USA (*03/09*) • Organizer of working group on "*Spin transitions in the lower mantle: the hidden transitions*", Workshop on Long Range Planning for High Pressure Earth Sciences, Tempe, AZ, USA (*03/09*) • Organizer/Instructor, ***VLab***/CIDER *Tutorial*, Kavli Institute for Theoretical Physics, Santa Barbara, USA (*07/08*). One week program within the Cooperative Institute for Deep Earth Research (CIDER) summer program • Organizer, ***VLab*** *Workshop*, Minnesota Supercomputing Institute, Minneapolis, USA (*07/05*), (*08/07*) • Organizer/Instructor, ***VLab****/ESPRESSO Tutorial*, Minnesota Supercomputing Institute, Minneapolis, USA (*05-06/06*). Offered for credit as a graduate course (MatS8995) • Topic Leader, *High Pressure Physics*, **APS** March Meeting, USA (*2006,2007,2008*) • Co-organizer of Focus sessions, *Earth and Planetary Materials*, **APS** March Meeting, Montreal (CA), Baltimore (USA) (*2004,2006*) • Organizer, Invited Symposium, *Computational Geophysics*, **APS** March Meeting, Austin, USA (*2003*) • Co-organizer, Topic Group *Materials Theory: Simulations*, **APS** March Meeting, San José, USA (*1996*) • Co-organizer, Symposium on *Perovskite Materials,* w/ Alexandra Navrotsky and Ken Poeppelmeier, **MRS** Spring Meeting, San Francisco, USA (*04/02*) • Co-organizer, Symposium on *High Pressure Materials Research*, w/ Peter Yu, Rus Hemley, and Bill Nellis, **MRS** Fall Meeting, Boston, USA (*12/97*) • Co-organizer, Symposium on *Materials Design and Modeling*, *V* International Conference on Advanced Materials, with Binglin Gu, Xianwei Sha, and Shuichi Iwata, **IUMRS** and **Chinese MRS**, Beijing, PRC (*12/99*) • Co-organizer, Symposium on *Frontiers in High Pressure Materials Physics*, Centre Européen de Calcul Atomique et Moléculaire (**CECAM**), with G. Chiarotti, K. Syassen, and R. Hemley, Lyon, France (*06/99*).

Research Funding

I have received US$9.0 M+ in funding from NSF and U of M since 1996. In 2004, I received a US$2.8M award to establish the Virtual Laboratory for Earth and Planetary Materials, ***VLab***, at the Minnesota Supercomputing Institute.

Current Grants:

- Theory of thermoelastic properties of iron-bearing minerals, PI R. Wentzcovitch, co-PI M. Cococcioni, NSF/EAR – 1319361, my part $336,001 (*08/13-07/16*).
- Collaborative Project – CSEDI: Integrated Study of H_2O in the Mantle, PI M. Hirschman, co-PIs D. Kohlstedt, R. Wentzcovitch, NSF/CSEDI - 1161023, $762,193 (my part $275,000) (*05/13-04/17 on no-cost extension*).
- U of M NSF/MRSEC, PI Tim Lodge, ~$240,000 in post-doc salary and fringe (*09/12-09/16*).
- Quantum Mechanical Modeling of Major Mantle Materials, PI Renata Wentzcovitch, co-PI David A. Yuen, NSF/EAR-1348066, $805,000 (my part $669,000) (*7/14-6/17*).
- Petascale Computations in Mineral Physics with the Quantum ESPRESSO, PI Renata Wentzcovitch, NSF/GLCPC, 3,000,000 CPU hours in the Blue Waters system.

• Collaborative Project – CSEDI – Understanding Fe and Si differentiation in the Earth's mantle and core through joint experimental and theoretical research in geochemistry and mineral physics - PI Nicolas Dauphas (U. of Chicago), co-PIs Renata Wentzcovitch (U of MN), Jung-Fu Lin (UT-Austin), NSF/EAR 1503084, my part $215,000 (05/01/15-04/30/18).

Teaching

- *Winter 1995, 1997, 1998* - Lecturer in ***Introduction to Materials Science*** **(MatS3600H)**. Honors class of the Institute of Technology at the junior level.
- *Spring 1996* - Lecturer in ***Electronic Structure of Materials*** **(MatS8214).** Graduate course on electronic structure at the CEMS Department.
- *Fall 1996, Spring 1999* - Lab instructor - *Fall 1997 and 1998*—Lecturer in ***Computational Methods in Chemical Engineering and Materials Science*** **(ChEn5001)** (four sessions). Undergraduate course in numerical methods applied to chemical engineering problems.
- *Fall 1999, 2000* - Lecturer - *Fall 2002* - Recitation instructor in ***Introduction to Materials Science and Engineering*** **(MatS3011)**. Large (150+ students) junior level class.
- *Spring 1998, 1999, 2001* - Lecturer in ***Introduction to Electrical and Magnetic Properties of Materials*** **(MatS5013)**. Senior level Materials Science course.
- *Spring 2000, Fall 2009*—Lecturer (*2000*) and recitation instructor (*2009*) in ***Materials and Energy Balances*** **(ChEn 4001)**. Large (180+ students) junior level class in the Chemical Engineering curriculum.
- *Spring 2002*—Lecturer of seminar series on ***Current Issues in Solid Earth Geophysics: Observations and First Principles Calculations*** at SISSA, Trieste, Italy.
- *Fall 2002, 2003*—Organizer of freshmen seminar ***Advances in Chemical Engineering and Materials Science and Engineering*** **(ChEn/MatS1001)**
- *Spring 2003, 2004, 2005, 2006, 2007, 2008*—Lecturer in ***Electronic Properties of Materials*** **(MatS8003).** Core graduate course in Materials Science.
- *Fall 2003* - Recitation instructor for ***Chemical Engineering Thermodynamics*** **(ChEn4101).** Junior level course in Chemical Engineering.
- *Fall 2004, 2006, 2015*—Lecturer and recitation instructor for ***Metals and Alloys*** **(MatS3012)** senior level course in Materials Science.
- *Summer 2006* - ***Vlab Tutorial in Computational Materials/Mineral Physics*** (**MatS8995)** (*05/21 to 06/03*). Educational outreach activity funded by NSF but also offered for credit to U of MN graduate students.
- *Fall 2007, 2010, 2011, 2012, 2013, 2014* - Lecturer and recitation instructor in ***Thermodynamics of Materials*** **(MatS4001/MatS3001)**, undergraduate course in Materials Science.
- *Fall 2009* - Recitation Instructor in ***Mass and Energy Balance*** **(ChEn2001)** junior level course in Chemical Engineering. Large (150+ students) junior level class.
- *Spring 2010* - ***Electronic Structure of Solids: Basic Theory and Practical Calculations*** **(MatS8223)**. I developed this in 2010. Introduces theoretical and computational methods for electronic structure calculations. Accompanied by hands-on computational labs that provide experience with the Quantum ESPRESSO software. It was designed having graduate students in CEMS, Physics, Chemistry, and engineering departments across CSE.
- *Spring 2011-13, 2016*—Recitations in ***Numerical Methods: Chemical Engineering Applications*** **(ChEn3201)**. Numerical analysis applied to ChemE problems.

- *Fall 2009, 2010, 2013, Spring 2011* - Organizer of ***Scientific Computation Seminar Series: Simulations in Materials and Chemistry*** **(SciC8190)** Weekly graduate seminars by U of MN faculty members in the Scientific Computation Program.
- *Spring 2014* - Recitations in ***Mass Transport and Kinetics*** **(MATS 3002)**. Undergraduate course in Materials Science.

Personnel Supervision

25 post-docs (5 currently), 9 graduate students (2 currently), 7 visiting graduate students (1 currently), 8 undergraduate students. 14 have permanent academic positions, 12 tenured.

Current Advisees: **Mehmet Topsakal,** research Assoc. (*09/13-*); **Pedro da Silveira** post-doc (*05/14-*)*;* **Kanchan Sarkar** Post-doc (*09/14-*); **Gaurav Shukla,** post-doc (*03/16-*); **Joelson Cott-Garcia,** post-doc (*09/15-*); **Juan Valencia-Cardona** Graduate student in Scientific Computing *(05/13-)*; **Tian Qin** (*07/14-*) Graduate student (Earth Sciences).

Michel Laderda Marcondes (*06/14-*) Visiting graduate student from Institute of Physics, University of São Paulo, SP, Brazil. **Chao Yao** (*09/15-*) Visiting graduate student from Department of Earth and Space Sciences—USTC-Hefei, PRC.

Past Advisees: **Wenhui Duan** (post-doc, *1996-99*) Prof., Physics, Tsinghua University, Beijing, PRC; **Cesar R. S. da Silva** (post-doc, *1996-99*, research Assoc., *2005-08*) Assoc. Prof., Department of Computer Science, Federal University of Uberlândia, MG, Brazil; **Bijaya Karki** (post-doc, *1997-2001*) Chair and Prof., Department of Computer Science and Engineering, Louisiana State University, Baton Rouge, LS, USA; **Koichiro Umemoto** (post-doc, *2003-06,* research Assoc., *2006-13*) Staff scientist, Earth and Life Sciences Institute, Tokyo Tech; **João Francisco Justo** (research Assoc., *2007-08*) Assoc. Prof., Electrical Engineering, Escola Politécnica, U. of São Paulo, SP, Brazil; **Taku Tsuchiya** (post-doc JSPS Fellow, *2003-05*) Prof., Center for Geodynamical Research, Ehime University, Japan; **Jun Tsuchiya** (post-doc JSPS Fellow, *2003-05*) Assoc. Prof., Center for Geodynamical Research, Ehime University, Japan; **Razvan Caracas** (post-doc, *2003-04*)**,** CR1 Researcher, CNRS, Laboratoire de Sciences de la Terre, École Normale Supérieure de Lyon, Lyon, France; **Amel Laref** (post-doc, *2006-07*) research Assoc., King Saud University, Department of Physics and Astronomy, Riyadh, Saudi Arabia; **Pierre Carrier (**research Assoc.**,** *2006-08*) Applications & benchmarking analyst, Cray Inc; **Zhongqing Wu** (post-doc, *2005-08*) Prof., Department of Earth and Space Sciences, U. of Science and Technology of China, Hefei, China; **Dipta Bahnu Ghosh** (post-doc, *2008-09*) research Assoc., Computer Science, LSU; **Han Hsu** (post-doc, *2007-11*) Asst. Prof., Physics Department, National Central University, Jhongli City, Taoyuan, Taiwan; **Tao Sun** (post-doc*, 2011-13*) Prof., Key Laboratory of Computational Geodynamics, University of the Chinese Academy of Sciences, Beijing, PRC. Winner of *1,000 Youth Talents of China* competition; **Dong-Bo Zhang** (post-doc*, 2011-14*) Assoc. Prof. of Computational Condensed Matter Physics, Computational Science Research Center, Chinese Academy of Engineering Physics, Beijing, PRC (*04/14*). Winner of *1,000 Youth Talents of China* competition; **Fawei Zheng** (post-doc, *2014-15)* Assoc. Prof., Computational Condensed Matter Physics, Institute for Applied Mathematics and Computational Physics, Chinese Academy of Engineering Physics, Beijing, PRC; **Kendall Thomson** (graduate student, *1995-99*) Assoc. Prof., Department of Chemical Engineering, Purdue University, West Lafayette, IN, USA; **Alexander Dobin (**graduate student, Physics, *1998-2001*, Graduated under Randall Victora) Scientific staff member at Cold Spring Harbor Laboratory, Cold Spring Harbor, NY, USA; **Chris Perrey** (graduate student, Materials Science, *1999-2001*, Graduated under Barry Carter) Principal Engineer at Tennant Company, Greater Minneapolis-St. Paul, MN, USA**; Yonggang Yu** (graduate student, Chemistry, *2004-08*,

Post-doc *2010-11*) *Winner of 2009 Graduate Research Award, Mineral and Rock Physics Group, AGU*; Humboldt Fellow in the Department of Geology, University of Frankfurt, Prof., Department of Earth Science, Nanjing University; Winner of *1,000 Youth Talents of China* competition; **Maribel Núnez-Valdéz** (graduate student, Physics *2009-11*, Post-doc *2011-12*). Post-doc, Department of Materials Science, ETH, Zürich, Switzerland (*2013-15*); Currently Research Assoc. at Moscow Institute of Physics and Technology (MIPT), Computational Materials Discovery Lab; **Pedro da Silveira** (graduate student, Scientific Computing, *2008-14*). Senior software analyst at Digital River and part time pot-doc with the Wentzcovitch group; **Gaurav Shukla** *(06/11-01/16)* Graduate student (Physics). Post-doc in CEMS with the Wentzcovitch group; **Elena Bernardis (**undergraduate student, Materials Science and Mathematics, *1999-2001*) Post-doc, Department of Radiology, U-Penn, Philadelphia, PA, USA; **Daniil Kigelman**, (undergraduate student, Computer Science, MSI/*VLab*, *2006-08*). Information Technology Professional, Thomson Reuters, Eagan, MN; **Neal Kelly** (undergraduate student, Materials Science, Mathematics and Computer Science, *2009-12*) (UMN -REU). Graduate student at Penn State, Materials Science; **Alexander Holiday** (undergrad student, Chemical Engineering, *2011-12*) (UMN-REU). Graduate student at Princeton University, Chemical Engineering; **Anne Carlson** (REU student, CEMS and Mathematics *2013-14*). **William R. Lindermann** (UMN/MRSEC-REU student from the Department of Materials Engineering, Iowa State University of Science and Technology, *2014*) Graduate student in Materials Science, MIT; **Caroline Qian** (UMN-REU student, CEMS and Computer Science, *2013-14*). **Blake Wolf** (*Summer'2015*) undergrad student (Materials Science). Graduate student at U of M (CEMS).

Visitors: **Victor Vinograd** (research Associate, Department of Geology, University of Frankfurt *04-06/10*). Research Scientist, Forschungszentrum Juelich GmbH, Juelich, Germany. **Ryan Requist** (graduate student from Physics and Astronomy, Stony Brook University *2006-07*. (advisor: Prof. Phil Allen)) Post-doc with Erio Tossatti at SISSA, Trieste, Italy. **Boris Kiefer** (graduate student from the Geological Sciences, University of Michigan, Ann Arbor (advisor: Prof. Lars Stixrude)) Associate Professor, Physics Department, University of New Mexico, NM, USA.

Publications

180+ papers published in peer reviewed journals, 17 conference proceedings; 3 books edited; one instruction video; Web of Science: 12,300+ citations; h-index 45; Google Scholar: 16,100+ citations; h-index 51; i10-index 144 (*05/2016*).

Edited Books

- *Theoretical and Computational Methods in Mineral Physics: Geophysical Applications, Reviews in Mineralogy and Geochemistry*, MSA, vol. 71 (2010), eds. R. M. Wentzcovitch & L. Stixrude.
- *Perovskite Materials*, Proceedings of Symposium D of the Materials Research Society Spring-02 Meeting, vol. 718 (2002), ed. by R. M. Wentzcovitch, A. Navrotsky, and K. Poeppelmeyer.
- *High Pressure Materials Research*, Proceedings of Symposium DD of the Materials Research Society, Fall-97 Meeting, vol. 499 (1998), ed. by R. M. Wentzcovitch, R. Hemley, W. Nellis, and P. Y. Yu.

Invited Presentations

Renata Wentzcovitch and group members have presented ~250+ invited talks and seminars since *1993*. Here are those from *01/2015*.

Workshops conferences

- "Plenary talk: New trends and recent achievements in theoretical high pressure research", 54th International Meeting of European High Pressure Group, Bayreuth, Germany (*09/16*).
- "Nature of the volume isotope effect in ice", (HPSP-17), Tokyo, Japan (*08/16*).
- "Spin crossover in ferropericlase and lateral velocity variations in the Earth's mantle", High Pressure Gordon Research Conference, Holderness, NH, USA (*07/16*).
- "High performance computing in mineral physics and materials science", National Academies of Science, Committee on Seismology and Geodynamics, Washington, DC (*04/16*).
- "Spin crossover in mantle minerals: some geophysical consequences", Workshop on "Next Generation Quantum Materials", ICTP-SAIFR, São Paulo, Brazil (*04/16*).
- "Spin crossover in mantle minerals", 2015 IUCr High-P Workshop, Campinas, Brazil (*09/15*).
- "Spin crossover in ferropericlase and lateral velocity variations in the Earth's mantle", Joint AIRAPT-EHPRG'2015 Conference, Madrid, Spain (*09/15*).
- "Key-Note Lecture: Spin crossover in ferropericlase and lateral velocity variations in the Earth's mantle", Symposium 25d: Physics and Chemistry of Earth Materials, Goldschmidt Conference, 25th Anniversary, Prague, Czeck Republic (*08/15*).
- "Spin crossover in (Mg,Fe)O", Symposium 4A: Advances in Computational Materials Science, XXIV International Materials Research Congress – Cancun, Mexico, (*08/15*).
- "Spin crossover in (Mg,Fe)O and implications for Earth's internal structure", Brazilian Physical Society Meeting, Foz do Iguaçu, Brazil (*05/15*).

Seminars and department colloquia

- "Spin Crossover in Iron Bearing Minerals", Center for Functional Materials, Brookhaven National Laboratory (*12/15*).
- "Modeling Earth Interior from Atomic to Global Scale", Geosciences, Stony Brook U. (*12/15*).
- "Modeling Earth Interior from Atomic to Global Scale", Institute for Advanced Computational Science, Stony Brook University (*12/15*).
- "The role of *Ab initio* Calculations in Geophysics", LDEO, Columbia University (*11/15*).
- "Modeling Earth Interior from Atomic to Global Scale", Department of Applied Physics and Applied Mathematics, Columbia University (*11/15*).
- "Spin Crossover in ferropericlase and lateral heterogeneities in Earth's lower mantle", Physics Department Colloquium, University of Toronto, Toronto, Canada (*10/15*).
- "Modeling Earth Interior from Atomic to Global Scale", Computational Science Research Center, Chinese Academy of Engineering Physics, Beijing, China (*06/15*).
- "Spin Crossover in ferropericlase and lateral heterogeneities in Earth's lower mantle", Physics Department, Tokyo-Tech, Tokyo, Japan (*01/15*).

Invited talks by recent group members

- *Koichiro Umemoto* - "Nature of the volume isotope effect in H_2O-ice", 2015 IUCr High-Pressure Workshop, Campinas, SP, Brazil (*09/15*).
- *Michel M. Lacerda* - "Hybrid *ab initio*-experimental approach to modeling thermal properties of solids", 2015 IUCr High-Pressure Workshop, Campinas, SP, Brazil (*09/15*).