RENATA M. M. WENTZCOVITCH
Professor of Applied Physics and Materials Science
Department of Applied Physics and Applied Mathematics
Department of Earth and Environmental Sciences
Lamont-Doherty Earth Observatory
Columbia University
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http://www.mineralscloud.com/

A. FIELD OF SPECIALIZATION

Materials Science and Engineering / Earth and Environmental Sciences with focus on:
• Computational Materials Physics
• Simulation of Matter at Extreme Conditions
• Mineral Physics

B. EDUCATION

Ph.D. in Physics	University of California, Berkeley, December (1988) Advisor: Marvin L. Cohen
M.Sc. in Physics (Magna cum Lauda)	University of São Paulo, Brazil *(1982)* Advisor: José Roberto Leite
B.Sc. in Physics	University of São Paulo, Brazil *(1980)*

C. PROFESSIONAL EXPERIENCE

1. Columbia University

• Professor, Department of Applied Physics and Applied Mathematics
• Professor, Department of Earth and Environmental Sciences, Lamont-Doherty Earth Observatory

2. University of Minnesota

• Professor, Department of Chemical Engineering and Materials Science *(2006-2016)*
• Additional affiliations:
- Member of the Graduate Faculty in the Chemical Physics Program
- Member of the Graduate Faculty in Earth Sciences
- Member of the Graduate Faculty in the School of Physics and Astronomy
- Member of the Graduate Faculty in the Scientific Computing Program

• Director of Graduate Studies, Scientific Computing Program, College of Science and Engineering *(2012-16)*
• Founding Director, Virtual Laboratory for Earth and Planetary Materials, Minnesota Supercomputing Institute *(2004-10)*
• Associate Professor, Department of Chemical Engineering and Materials Science *(2001-06)*
• Assistant Professor, Department of Chemical Engineering and Materials Science *(1994-2001)*

2. Post-doctoral Appointments

• Research Fellow, Department of Geological Sciences, University College London, and The Royal Institution of Great Britain, London, UK, with David G. Price, *(1993-94)*
• Theory of Condensed Matter Group (TCM), Cavendish Laboratory, Cambridge, UK, with Volker Heine *(1992-93)*

• Department of Physics, Brookhaven National Laboratory, and Department of Physics, Stony Brook University, with Philip B Allen *(1989-92)*

3. Affiliations with Other Institutions

• Adjunct Research Scientist, Lamont Doherty Earth Observatory, Columbia University (*08/2016-01/2017*)

• Principle Investigator at the Earth-Life Science Institute (ELSI), World Premier International Research Institute (WPIRI) of the JSPS, Tokyo Institute of Technology, Tokyo, Japan *(10/2012-2016).* Associate Investigator (*2017*-)

• Visiting Professor, Computational Science Research Center, Chinese Academy of Engineering Physics, Beijing, China *(06/2015, 10-11/2016).*

• Visiting Professor, Department of Earth and Space Sciences, University of Science and Technology of China, Hefei, China *(07/2012, 8/2013).*

• Visiting Professor, Faculty of Sciences, Interactive Center for Science, Tokyo Institute of Technology, Tokyo, Japan *(5/2010-8/2010)*

• Visiting Professor, Departments of Physics and Earth and Planetary Sciences, Tokyo Institute of Technology, Tokyo, Japan *(04/2002, 08/2006, 10-12/2008)*

• Visiting Professor, Departments of Geology, University of Frankfurt, Germany *(09/2008-11/2008, 08/2009, 08/2010, 08/2012)*

• Visiting Professor Department of Physics and Astronomy and Department of Geological Sciences, (*Fall* 2005) and Department of Physics and Astronomy *(08/1995, 02/1996, 08/1997, 07/1998)*, Stony Brook University, Stony Brook, NY, USA .

• Distinguished Visiting Professor (*2005*), Visiting Professor *(08/2001, 08/2002, 08/2003, 08/2004, 08/2012, 08/2017)* and Visiting Scientist *(08/1998, 08/1999, 08/2000)*, Scuola Internazionale Superiori di Studi Avanzati, SISSA, Trieste, Italy

• Visiting Scientist, National Institute for Computer Science and Engineering, INESC, Lisbon, Portugal, *(01/1996)*

• Assistant Professor, Department of Materials Physics, Institute of Physics, University of São Paulo, Brazil *(1995-96)*

• Visiting Researcher, The James Franck Institute, University of Chicago *(Fall 1988)*

D. TEACHING EXPERIENCE

1. Courses taught at Columbia University

• *Spring 2018, 2019* – Lecturer in *Electronic Structure of Complex Materials* (MSAE E6085). Graduate course on theoretical and computational methods in electronic structure (class size, ~10 students).

• *Spring 2019* – Lecturer in *Introduction to Materials Science* (MSAE E3011). Junior level course on introductory Materials Science (class size, ~10 students).

2. Courses taught at the University of Minnesota

• *Winter 1995, 1997, 1998* - Lecturer in *Introduction to Materials Science* (MatS3600H). Honors class of the Institute of Technology at the junior level (medium size class, 40 students).

• *Spring 1996* - Lecturer in *Electronic Structure of Materials* (MatS8214). Graduate course in electronic structure (small class, 5 students).

- *Fall 1996, Spring 1999* - Lab instructor - *Fall 1997 and 1998* – Lecturer in *Computational Methods in Chemical Engineering and Materials Science* (ChEn5001) (four sessions, 25 students each). 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). Junior level course (large class, 150+ students).
- *Spring 1998, 1999, 2001* - Lecturer in *Introduction to Electrical and Magnetic Properties of Materials* (MatS5013). Senior level Materials Science course (medium size class, 30 students).
- *Spring 2000, Fall 2009* – Lecturer (2000) and recitation instructor (*2009*) in *Materials and Energy Balances* (ChEn 4001). Junior level course in the Chemical Engineering curriculum (large class, 180+ students).
- *Fall 2002, 2003* – Organizer of freshmen seminar *Advances in Chemical Engineering and Materials Science and Engineering* (ChEn/MatS1001) (medium size, 60 students).
- *Spring 2003, 2004, 2005, 2006, 2007, 2008* – Lecturer in *Electronic Properties of Materials* (MatS8003). Core graduate course in Materials Science (medium size, ~30 students).
- *Fall 2003* - Recitation instructor for *Chemical Engineering Thermodynamics* (ChEn4101). Junior level course in Chemical Engineering (medium/large size class, 60+ students).
- *Fall 2004, 2006, 2015* – Lecturer and recitation instructor for *Metals and Alloys* (MatS3012) senior level course in Materials Science (medium/large size class, 60+ students)..
- *Summer 2006 - Vlab Tutorial in Computational Materials/Mineral Physics* (MatS8995) (*05/21 to 06/03*). Educational outreach activity supported by NSF but also offered for credit to U of MN graduate students (medium size class, ~40 students). This course is available online: http://www.mineralscloud.com/events/lecture.shtml
- *Fall 2007, 2010, 2011, 2012, 2013, 2014* - Lecturer and recitation instructor in *Thermodynamics of Materials* (MatS4001/MatS3001), junior level undergraduate course in Materials Science (medium/large size class, ~40-70 students).
- *Fall 2009* - Recitation Instructor in *Mass and Energy Balance* (ChEn2001) junior level course in Chemical Engineering (large class 150+ students).
- *Spring 2010 - Electronic Structure of Solids: Basic Theory and Practical Calculations* (MatS8223). Graduate course I developed in 2010. This course introduces theoretical and computational methods for electronic structure calculations. It is 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 (small class, 7 students).
- *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 (~20 students).
- *Spring 2011, 2012, 2013, 2014, 2016* - Recitations in *Numerical Methods: Chemical Engineering Applications* (ChEn3201). Junior level course in numerical methods applied to chemical engineering problems (4 sessions, 25 students each).

2. Courses taught at other institutions

• *Summer (2001) - Current Topics in Solid Earth Geophysics: Observations and First Principles Calculations*, SISSA, Trieste, Italy. One month course with 2 classes per week. Small class (~10 students).

• *Summer (2015) - Theoretical and Computational Methods in Mineral Physics,* Institute of Physics, University of São Paulo, SP, Brazil. Two weeks course with 3 classes per week. Small class (~10 students).

3. Personnel Supervision

• *Current Advisees*

Columbia University

Michel Marcondes-Lacerda (05/2017-) Research Associate, Lamont-Doherty Earth Observatory.

Kanchan Sarkar (09/2017-) Post-doc in the Department of Applied Physics and Applied Mathematics.

Zhen Zhang (09/2017-) Graduate student (PhD track), Department of Applied Physics and Applied Mathematics, Applied Physics Program.

Qi Zhang (02/2017-) Graduate student (MSc track until *08/2018*, PhD track starting on *09/2018*) in the Department of Applied Physics and Applied Mathematics, Materials Science Program.

Tianqi Wan (06/2018-) Graduate student (MSc track) in the Department of Applied Physics and Applied Mathematics, Materials Science Program.

Hongjin Wang (06/2018-) Graduate student (MSc track) in the Department of Applied Physics and Applied Mathematics, Materials Science Program.

Jingyi Zhuang (06/2018-) Graduate student (MSc track) in the Department of Applied Physics and Applied Mathematics, Materials Science Program.

Ziyu Cai (06/2018-) Graduate student (MSc track) in the Department of Applied Physics and Applied Mathematics, Materials Science Program.

Chenxing Luo (06/2018-) Graduate student (MSc track) in the Department of Applied Physics and Applied Mathematics, Materials Science Program.

University of Minnesota

Tian Qin (07/2014-) Graduate student (PhD track) in the Department of Earth Sciences.

• *Alumni: Post-doctoral fellows*

Wenhui Duan (*1996-99*) Currently Professor, Physics Department, Tsinghua University, Beijing. Fellow of Chinese Academy of Sciences (*2016*), China.

Cesar R. S. da Silva (CNPq Fellow, *1996-99,* and Research Associate, *2005-2008*) Currently Associate Professor, Department of Computer Science, Federal University of Uberlândia, MG, Brazil.

*Bijaya Kark*i (*1997-2001*) Currently Chair and Professor, Department of Computer Science and Engineering, Louisiana State University, Baton Rouge, LS, USA.

Koichiro Umemoto (*2003-06*, research associate, *2006-13*) Currently staff scientist, Earth-Life Science Institute, TITech, Tokyo, Japan.

João Francisco Justo (research associate, *2007-08*) Associate Professor, Electrical Engineering, Escola Politécnica, U. of São Paulo, SP, Brazil.

Taku Tsuchiya (JSPS Fellow, *2003-2005*) Professor of Mineral Physics, Center for Geodynamical Research, Ehime University, Japan.

Jun Tsuchiya (JSPS Fellow, *2003-05*) Associate Professor, Center for Geodynamical Research, Ehime University, Japan.

Razvan Caracas (*2003-04*), CR1 Researcher, CNRS, Laboratoire de Sciences de la Terre, École Normale Supérieure de Lyon, Lyon, France.

Amel Laref (*2006-07*) Research Associate, King Saud University, Department of Physics and Astronomy, Riyadh, Saudi Arabia.

Pierre Carrier (*2006-08*) Applications and benchmarking analyst, Cray Inc., Minnerapolis, MN, USA.

Zhongqing Wu (*2005-08*) Professor, Department of Earth and Space Sciences, U. of Science and Technology of China, Hefei, China.

Dipta Bahnu Ghosh (*2008-09*) Research Associate, Department of Computer Science, LSU.

Han Hsu (*2007-11*) Assistant Professor, Physics Department, National Central University, Jhongli City, Taoyuan, Taiwan.

Yonggang Yu (*2010-11*) *Winner of 2009 Graduate Research Award, Mineral and Rock Physics Group, AGU*; Humboldt Fellow in the Department of Geology, University of Frankfurt, Professor of Mineral Physics, Department of Earth Science, Nanjing University, Nanjing, CN (*2013)*; Winner of *1,000 Youth Talents of China* competition. Currently staff member at NOAA, Earth System Research Lab, Global Systems Division, Boulder, CO, USA.

Maribel Núnez-Valdéz (*2011-13*) W2-Professor, Helmholtz-Zentrum, Deutsches GeoForschungsZentrum (GFZ), Potsdam, Germany.

Tao Sun (*2011-13*) Professor of Mineral Physics, Key Laboratory of Computational Geodynamics, University of the Chinese Academy of Sciences, Beijing, China. Winner of *1,000 Youth Talents of China* competition.

Dong-Bo Zhang (*2011-14*) Associate Professor of Computational Condensed Matter Physics, Computational Science Research Center, Chinese Academy of Engineering Physics, Beijing, China (*04/14*). Winner of *1,000 Youth Talents of China* competition.

Fawei Zheng (post-doc, *2014-15)* Associate Professor, Computational Condensed Matter Physics, Institute for Applied Mathematics and Computational Physics, Chinese Academy of Engineering Physics, Beijing, China.

Mehmet Topsakal (2013-16) Research Associate, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY, USA.

Gaurav Shukla (*2016*) post-doc in the Department of Earth, Ocean, and Environmental Sciences, Florida State University, Tallahassee, FL, USA.

Pedro da Silveira (*2014-16)* Senior software engineer, Digital River, Minnetonka, MN, USA

Joelson Cott-Garcia (2016) Business/Materials Development Researcher, Nissan Chemical America Corporation, Santa Clara, CA, USA.

Kanchan Sarkar (09/2014-17) Post-doc in Materials Science.

• *Alumni: Graduate students*

Kendall Thomson (PhD, Chemical Engineering, *1995-99*) Currently Associate Professor, Department of Chemical Engineering, Purdue University, West Lafayette, IN, USA.

*Alexander Dobin (*PhD, Physics, *1998-2001*. Graduated under Randall Victora. *Currently* scientific staff member at Cold Spring Harbor Laboratory, Cold Spring Harbor, NY, USA.

Chris Perrey (PhD, Materials Science, *1999-2001*) Graduated under Barry Carter, Currently, Principal Engineer at Tennant Company, Minneapolis-St. Paul, MN, USA.

Yonggang Yu (PhD, Chemistry). Currently staff member at NOAA, Earth System Research Lab, Global Systems Division, Boulder, CO, USA.

Maribel Núnez-Valdéz (PhD, Physics *2009-11*). W2-Professor, Helmholtz-Zentrum, Deutsches GeoForschungsZentrum (GFZ), Potsdam, Germany.

Pedro da Silveira (PhD graduate student, Scientific Computing *2008-14*). Currently, senior software engineer, Apple Inc., Austin, TX.

Gaurav Shukla (PhD, Physics, *2011-15*) Assistant Professor of Earth Sciences, Indian Institute of Science, Education, and Research (IISER), Kolkata, India.

Juan Valencia-Cardona (PhD, Scientific Computing Program, *2014-18.* Currently, Computer Aided Design Engineer, Intel, Seattle, WA.

• *Alumni: Undergraduate students*

Blake Wolf - Materials Science, CEMS *(Summer 2015)*. Currently a graduate student in Materials Science and Electrical Engineering, University of Minnesota, MN, USA.

William R. Lindemann - Department of Materials Engineering, Iowa State University, UMN/MRSEC-REU student from the (*Summer 2014)*. Currently a graduate student in Materials Science, MIT, Boston, USA.

Caroline Qian - Chemical Engineering (CEMS) and Computer Science, UMN-REU student (*01-12/2014)*. Currently a graduate student in Chemical Engineering, UC-Irvine, CA, USA.

Anne Carlson Chemical Engineering (CEMS) and Mathematics, UMN-REU student (*01-12/2013)*. Currently at Cortec Corporation, Minneapolis, MN, USA.

Rajat Ghosh - Chemical Engineering (CEMS) (*06-12/2014)*. Currently a modeler at ExxonMobil, Houston, TX, USA.

Alexander Holiday - Chemical Engineering, CEMS, UMN-REU student (*2011-12*). Currently a graduate student, Chemical Engineering, Princeton University, NJ, USA.

Neal Kelly - Materials Science, Mathematics, and Computer Science, UMN-REU student (*2009-12*). Currently a software developer and database manager, UnitedHealth Group, Minneapolis, MN, USA.

Daniil Kigelman - Computer Science, intern at the Minnesota Supercomputing Institute (*2006-08*). Software developer and database manager, Thomson Reuters, Eagan, MN, USA.

Elena Bernardis - Materials Science and Mathematics, CEMS, UMN-REU student (1999-2001). PhD in Computer Science (medical imaging), U-Penn. Currently a Research Associate, Children's Hospital of Philadelphia, PA, USA.

• *Alumni: Visiting students and researchers*

Chao Yao - Graduate student from School of Earth and Space Sciences – USTC-Hefei, China, with Prof. Zhongqing Wu *(2015-16)*. Currently a graduate student at USTC.

Michel Lacerda Marcondes dos Santos - Graduate student from Institute of Physics, University of São Paulo, SP, Brazil, with Prof. Lucy C. Assali *(2014-15)*. Currently, a post-doc at Airforce Technology Institute (ITA), São José dos Campos, SP, Brazil.

Yuichiro Yamagami - Graduate student from Physics, Tokyo Institute of Technology, with Prof. Susumu Saito (*2009*). He moved to the private sector, Tokyo, Japan.

Victor Vinograd - Research Associate from the Department of Geology, University of Frankfurt *(Summer 2010*). Research Scientist, Forschungszentrum Juelich GmbH, Juelich, Germany.

Tao Sun - Graduate student from Physics and Astronomy, Stony Brook University, with Prof. Philip B. Allen (*2007-08)*. Currently Associate Professor of Mineral Physics, Key Laboratory of Computational Geodynamics, University of Chinese Academy of Sciences, Beijing, China.

Di Wang - Graduate student from the Department of Geophysics, Virginia Tech with Prof. Nancy Ross (*Summer 2009)*. Currently software developer at CGG, Houston, TX, USA.

Ryan Requist - Graduate student from Physics and Astronomy, Stony Brook University, with Prof. Philip B Allen (*2006-07)*. Research Associate, Max Planck Institute-Halle, Germany.

Gilberto Paiva - Graduate student from the Materials Department, University of São Paulo, with Prof. Adalberto Fazzio (*1997-98).* Currently a high school teacher, São Paulo, Brazil.

Boris Kiefer - Graduate student from Geological Sciences, University of Michigan, Ann Arbor, with Prof. Lars Stixrude (*1997).* Currently Associate Professor, Physics Department, University of New Mexico, NM, USA.

E. HONORS AND AWARDS

- Vice-Chair, Chair-Elect, Chair, Past-Chair, Division of Computational Physics, American Physical Society (*2017-20*)
- Wilhelm Heraeus Visiting Professorship Award, University of Frankfurt (€40,000) (*2015-16*)
- Fellow, American Academy of Arts and Sciences (*2013*-)
- Fellow, American Association for Advancement of Science (Physics) (*2012*-)
- Fellow, Mineralogical Society of America (*2009*-)
- Fellow, American Geophysical Union (*2008*-)
- Fellow, American Physical Society, Division of Materials Physics (*2006*-)
- Alexander von Humboldt Research Award for Senior US Scientists (€60,000) (*2008*)
- Japan Society for Progress of Science (JSPS), Invitation Fellowship for Research in Japan (*2008*)
- Member at-large, American Physical Society, Division of Computational Physics (*2000-03*)
- Fellow (*2001*-) and Associate Fellow (*1997-2001*) of Minnesota Supercomputing Institute
- Shell Land-Grant Professor in Chemical Engineering and Material Science, University of Minnesota (*1994-95*)
- Honorary Research Fellow, Birkbeck College, University of London, UK (*1993-94*)
- Fellowships from Brazilian agencies:

- São Paulo State Research Foundation, FAPESP (undergraduate, *1978-80*), with Sueli Aldrovandi (Astrophysics, Institute for Astronomy and Geophysics, University of São Paulo)
- National Research Council for Nuclear Energy, CNEN (MSc, *1980-82*), with José Roberto Leite (Physics, Nuclear Energy Research Institute, University of São Paulo)
- National Research Council, CNPq (PhD, *1983-87*) with Marvin L. Cohen (Physics, UC-Berkeley)

Awards to Advisees

• Graduate Research Award of the Mineral and Rock Physics Group, AGU (*2009*), PhD thesis of graduate student Yonggang Yu
• Outstanding Student Paper Award of the Mineral and Rock Physics Group, AGU (*2009*) to graduate student Maribel Núnez-Valdez.

F. CONFERENCES, WORKSHOPS, TUTORIALS, AND SPECIAL SESSIONS ORGANIZED

1) Program Chair of the Division of Computational Physics, APS March Meeting 2019, Boston. 130+ sessions. (*03/2019*).

2) Organizer of Invited Session at the APS 2019 March Meeting: *Physics of Planetary Interiors: Modeling Planets from Atomic to Global Scale*, Boston. (*03/2019*).

3) Organizer of Invited Session at the APS 2019 March Meeting: *Materials at Tera Pascals: a New Frontier in Materials Theory and Simulations*, Boston. (*03/2019*).

4) Co-organizer, Mineral and Rock Physics Sessions, *Advances in Computational Mineral Physics and Geochemistry*, American Geophysical Union Fall'18 Meeting, Washington DC. (*12/2018*).

5) Co-organizer with lead-organizer Marcos Rigol and Chris Van de Walle of 113 sessions sponsored and co-sponsored by the Division of Computational Physics, at the APS March Meeting 2018, Los Angeles. (*03/2018*).

6) Co-organizer, Mineral and Rock Physics Sessions, *Mineral physics at ultrahigh pressures: Giant planets, exoplanets, and giant impacts*, American Geophysical Union Fall Meeting, New Orleans, USA *(12/2017).*

7) Lead organizer, with co-organizer Alexandra Navrotsky, Breakout Session: *Infrastructure for Computational and Theoretical Mineral Physics*, for Consortium on Materials Properties Research in Earth Sciences, COMPRES Meeting (*06/2016*).

8) Lead organizer, with co-organizers Liliana Arrachea (AR), Eduardo Miranda (BR), and Richard Martin (USA)), Workshop: *Next Generation Quantum Materials*, International Center for Theoretical Physics, South American Institute for Fundamental Research (ICTP-SAIFR), São Paulo, Brazil (*04/2016*).

9) Instructor of Mini-Course: *Ab Initio Modeling of Materials at Extreme Conditions*, Department of Materials Physics, University of São Paulo, Brazil (*05/2015*).

10) Organizer: Computational Approaches in High Pressure Research, High Pressure Workshop of the International Union of Crystallography, Campinas SP, Brazil (*09/2015*)

11) Lead organizer, with co-organizer David Bercovici, Symposium: *Modeling Earth's Interior from Atomic to Global Scale*, American Association to Advancement of Science Annual Meeting, San José, CA, USA *(02/2015)*.

12) Instructor of Mini-Course: *Ab Initio Modeling of Materials at Extreme Conditions*, Department of Materials Physics, University of São Paulo, Brazil (*05/2015*).

13) Lecturer and instructor of computational labs at the African School of Electronic Structure Methods and Applications, ASESMA**,** (two week program): African Institute for Mathematical Sciences, Cape Town, South Africa (*07/2010*); Chepkoilel College, Eldoret, Kenya *(05/2012)*.

14) Co-organizer, Mineral and Rock Physics Sessions, *The role of transition elements in geophysical and geochemical processes in the deep Earth*, American Geophysical Union Fall Meeting, San Francisco, USA *(2014).*

15) Co-organizer, Mineral and Rock Physics Sessions, *Thermodynamic & Elasticity Databases and the Geoinformatics Revolution: Objectives, Scope and Construction of Data Systems for Geochemical and Geophysical Modeling*, American Geophysical Union Fall Meeting, San Francisco, USA *(2013).*

16) Co-organizer, Mineral and Rock Physics Sessions, *Electronic and Elastic properties of Mantle Materials*, American Geophysical Union Fall Meeting, San Francisco, USA *(2012).*

17) Lead-organizer, with Don Truhlar, *Symposium: Quantum chemistry meets geochemistry*, 243rd American Chemical Society National Meeting, San Diego, USA *(03/2012).*

18) Co-organizer, Mineral and Rock Physics Sessions, *Deep Mantle Properties*, Fall American Geophysical Union Meeting, San Francisco, USA *(2010).*

19) Co-organizer, Mineral and Rock Physics Sessions, *Recent Advances in Understanding Dynamics, Structure, and Composition of the Deep Lower Mantle*, Joint Assembly, Spring American Geophysical Union Meeting, Toronto, Canada *(2009).*

20) Co-organizer, Mineral and Rock Physics Sessions, *Spin Crossover Transitions in the Lower Mantle*, American Geophysical Union Fall Meeting, San Francisco, USA *(12/08),*

21) Co-organizer, Mineral and Rock Physics Sessions, *Computational Mineral Physics*, American Geophysical Union Spring Meeting (*2006*), Baltimore, and Fall Meeting in San Francisco (USA) *(2007,2008,2009).*

22) Co-organizer, Mineral and Rock Physics Sessions, *Post-perovskite Phase Transition and the D" Layer*, American Geophysical Union, Fall Meeting, San Francisco, USA *(2004).*

23) Organizer, "*Infrastructure for Computational Mineral Physics: a Community Consultation Workshop"*, Consortium on Materials Properties Research in Earth Sciences, COMPRES (*08/2010*). Co-author of *"Infrastructure for Computational Mineral Physics: a Community Consultation Workshop"*, COMPRES report to the National Science Foundation.

24) 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 *(10/2010).*

25) Organizer, "*Theoretical and Computational Methods in Mineral Physics: Geophysical Applications*", Joint Short Course for the Mineralogical Society of America and ***VLab***, Berkeley CA, USA *(03/2009).*

26) Organizer of working group on "*Spin transitions in the lower mantle: the hidden transitions*" , Workshop on Long Range Planning for High Pressure Earth Sciences, Consortium on Materials Properties Research in Earth Science, COMPRES, Tempe, AZ, USA *(03/2009).*

27) Organizer/Instructor, ***VLab***/CIDER *Tutorial*, Kavli Institute for Theoretical Physics, Santa Barbara, USA. One week program within the Cooperative Institute for Deep Earth Research, CIDER, (*Summer 2008*).

28) Organizer, ***VLab*** *Workshop*, Minnesota Supercomputing Institute, Minneapolis, USA (*07/2005*), (*08/2007*).

29) Organizer/Instructor, ***VLab****/ESPRESSO Tutorial*, Minnesota Supercomputing Institute, Minneapolis, USA (*05-06/2006*). Offered for credit as a graduate course (MatS8995).

30) Topic Leader and Lead-organizer, *High Pressure Physics*, American Physical Society, March Meeting, USA (*2006,2007,2008*).

31) Organizer of Focus sessions, *Earth and Planetary Materials*, American Physical Society, March Meeting, Baltimore (USA) (*2006*).

32) Organizer of Focus sessions, *Earth and Planetary Materials*, American Physical Society, March Meeting, Montreal, CA (*2004*).

33) Organizer, Invited Symposium, *Computational Geophysics*, American Physical Society, March Meeting, Austin, USA (*2003*).

34) Co-organizer, Topic Group *Materials Theory: Simulations*, with James Chelikowsky, American Physical Society, March Meeting, San José, USA (*1996*).

35) Co-organizer, Symposium on *Perovskite Materials*, with Alexandra Navrotsky and Ken Poeppelmeier, Materials Research Society Spring Meeting, San Francisco, USA *(2002).*

36) Lead-organizer, Symposium on *High Pressure Materials Research*, w/ Peter Yu, Rus Hemley, and Bill Nellis, Materials Research Society Fall Meeting, Boston, USA (*1997*).

37) Co-organizer, Symposium on *Materials Design and Modeling, V* International Conference on Advanced Materials, with Bing Lin Gu, Xianwei Sha, and Shuichi Iwata, International Union of Materials Research Society with and Chinese Materials Research Society, Beijing, China *(12/1999).*

38) Co-organizer, Symposium on *Frontiers in High Pressure Materials Physics*, Centre Européen de Calcul Atomique et Moléculaire (CECAM), with Guido Chiarotti, Karl Syassen, and Rus Hemley, Lyon, France (*06/1999*).

39) Organizer of the Department of Chemical Engineering and Materials Science Seminar Series, University of Minnesota *(1996, 2007).*

J. SERVICE

1. Service to Columbia University

• *General*

- Columbia University representative in the Board of Directors of the Great Lakes Consortium for Petascale Computing – The Blue Waters Project (*2017*-)
- Data Science Institute - member of "Frontiers in Computing Systems" working group.

• *APAM Department*

- APAM Research Conference Organizer (*Fall-2017, Fall-2018*) a weekly series of seminars by Columbia faculty members, primarily from the School of Engineering and Applied Sciences
- Director: "Materials Theory and Simulation" Concentration Area in the Materials Science MSc program

• *Department of Earth and Environmental Sciences*

- Faculty Recruiting Committee (*Spring-2018*)
- Under Represented Minority Faculty Recruiting Committee (*Spring-2019*)

2. Service to the University of Minnesota

• *General*

-Director of Graduate Studies, Scientific Computation Program, College of Science and Engineering (*2012-16*)

-Faculty Recruiting Committee, Department of Earth Sciences (*2014*) Office of the Vice-President for Research, Grant-in-Aid for Research and Scholarship review panel *(2013, 2014)*

-University of Minnesota Point-of-Contact for the University of Minnesota/Tokyo Institute of Technology Cooperation in Graduate Education Program (*2013-16*)

-University of Minnesota representative and elector to the Consortium on Materials Proeprties Research in Earth Sciences (COMPRES), National Science Foundation (*2003-16*)
-Basic Sciences Computing Laboratory Steering Committee (*2000-01*)
-President's Distinguished Faculty Mentor Program *(1998-2001)*
-Institute of Technology's Instructional Computing Committee *(1999-00)*

• *CEMS Department (U of MN)*
-Graduate Recruiting Committee *(1994,2005,2006,2011, 2012)*
-Faculty Recruiting Committee *(2005)*

• *Minnesota Supercomputing Institute*
-Allocation Committee (*2009-2012*), Chair (*2009-10*)
-Founding Director, Virtual Laboratory for Earth and Planetary Materials, *VLab,* Minnesota Supercomputing Institute, U of MN (*2004-10*)
-Digital Technology Center and Minnesota Supercomputing Institute Task Force on Initiatives in High Performance Computing *(2006-07)*
-Long-range Planning Committee *(2006-07)*
-Research Scholarship Committee *(2003-06,* Chair in *2006)*
-Nominating Committee *(1997-99,2001-03)*
-IBM-SP Advisory Committee *(1997-98)*

3. Service to the discipline

• *Society memberships*:
-American Physical Society (Fellow in *2005*) (APS), American Geophysical Union (AGU) (Fellow in *2008*), Mineralogical Society of America (Fellow in *2009*), American Association for the Advancement of Science (Fellow in *2012)* (AAAS), Materials Research Society (MRS), American Chemical Society (ACS).

• *Service to the American Physical Society (APS):*
-Vice-Chair (*2017*), Chair-Elect (*2018*), Chair (*2019*), Past Chair (*2020*), Division of Computational Physics (APS/DCOMP)
-Aneesur Rahman Prize Fundraising Committee (*2019-*)
-APS March Meeting, DCOMP Program Chair *(2019)*
-APS/DCOMP March Meeting Program Committee *(2002-03)*
-Chair, APS/DCOMP International Liaison Committee (*2017*)
-DCOMP - Aneesur Rahman Prize selection Committee, Vice-Chair *(2012*), Chair (*2016*)
-Fellows Nominating Committee - member (*2008-11*)
-DCOMP - Executive Committee (Member at-large) (*2000-03*)
-APS March Meeting Program Committee *(2003)*
-Committee on the Status of Women in Physics, site visit team member to U. of Washington *(2005)*

• *Service to the International Association for High Pressure Research, AIRAPT*
-Bridgman Prize Selection Committee (*2009*)
-27th International Conference on High Pressure Science and Technology, Rio de Janeiro, Brazil (*2019*), International Advisory Committee and Program Committee member

• *Consortium on Materials Properties Research in Earth Sciences, COMPRES,*
-Long range planning committee (*2010*)

-Co-author of NSF report: *"Understanding the Building Blocks of the Planet: The Materials Science of Earth Processes"* (*2010*)

• *Review Panels:*

-Department of Energy (DOE/BES)**:** Review panel member for the Condensed Matter Physics Program at Ames Laboratory *(2018)*

-National Science Foundation: XSEDE's 2nd Annual review panel *(2013)*

-Department of Energy: Review panel member for the Energy Frontier Research Center, High Pressure Energy Research in Extreme Environments, Carnegie Institution of Washington, Geophysical Laboratory *(2012)*

-Department of Energy**:** Review panel member for the Energy Frontier Research Center, Center for Emerging Superconductivity, BNL/ANL/UIUC *(2012)*

-National Science Foundation**:** Review panel member for OCI/SI2 Software Institutes *(2012)*

-Department of Energy**:** Review panel member for the Theoretical Chemical Physics Program at Pacific Northwest Laboratory *(2010)*

-National Science Foundation: High Performance Computing (track 2b) *(2006,2009)*

-Joint National Science Foundation and Deutsche Forschungsgemeinschaft, Materials Research Review Panel, Materials World Network - Berlin (*2007*)

-National Science Foundation: Materials World Network: Cooperative Activity in Materials Research between US Investigators and their Counterparts Abroad (MWN) *(2007)*

-National Science Foundation: Arizona State University MRSEC *(1999)*

• *Editorial Service*

-Associate Editor *Journal of Physics: Condensed Matter, Electronic Structure*, a new journal of IOP Publishing (Bristol, UK) launched on *3/2018*.

-Associate Editor, *The American Mineralogist*, Mineralogical Society of America (*2011-16*)

• *Regular referee services:*

-American Physical Society, American Chemical Society, Materials Research Society, American Geophysical Union, National Academy of Sciences publications, Nature and Science series publications, Journal of Physics Condensed Matter, European Physics Letters primarily.

-Funding agencies: US National Science Foundation, Department of Energy, Petroleum Research Fund, UK Science and Engineering Research Council (SERC) and Natural Environment Research Council (NERC), Germany's Deutsche Forschungsgemeinschaft (DFG), Italian Ministry of Education, University and Research (MIUR), Japan Society for Promotion of Science (JSPS), and Swiss National Science Foundation.

• *External PhD defense committees*

-*Di Wang* –Thesis Title: "Some Aspects of the Crystal Chemistry of Perovskites", PhD in Geology, Virginia Tech *(06/12)*

-*Brian Boates* –Thesis Title: "On the Stability of SP-Materials at High Pressure", PhD in Physics, Dalhousie University, Halifax, Canada *(09/12)*

-*Swastika Chatterjee* - Thesis Title: "First Principles Study of Silicate Minerals", PhD in Physics, University of Calcutta *(02/13)*

-*Richard Charles Andrew* –Thesis Title: "First Principles Studies of Si-C Alloys", PhD in Physics, University of Pretoria, Pretoria, South Africa *(03/13)*

E. PUBLICATIONS

1. BOOKS EDITED

1. **Theoretical and Computational Methods in Mineral Physics: Geophysical Applications**, *Reviews in Mineralogy and Geochemistry, Mineralogical Society of America,* vol. **71** (2010), ed. by R. M. Wentzcovitch, and L. Stixrude. Online: http://rimg.geoscienceworld.org/current.dtl
2. **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.
3. **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.**

2. JOURNAL PUBLICATIONS

200+ publications in peer reviewed journals, 18 conference proceedings; 3 books edited; one instruction video; Web of Science: 18,600+ citations; h-index 50; Google Scholar: 25,100+ citations; h-index 59; i10-index 161 (*03/2019*).

2019

203. C. Houser, J. Hernlund, J. Valencia-Cardona, and R. Wentzcovitch, **Limitations of global 1D seismic model comparisons to constrain lower mantle composition**, *Phys. Earth. & Planet. Int*., in press (2019).
202. K. Umemoto and R. M. Wentzcovitch, **First principles investigation of post-PPV transitions in low-pressure analogs of $MgSiO_3$**, *Earth & Planet Sc. Lett*., in press (2019).
201. G. Shukla, K. Sarkar, and R. M. Wentzcovitch, **Thermoelastic properties of Al- and Fe-bearing post-perovskite**, *J. Geophys. Res.*, in press (2019).
200. J. Tromp, M. L. Marcondes, R. M. Wentzcovitch, and J. Trampert**, Effect of induced stress on seismic waves: validation based on *ab initio* calculations,** *Geophys. J. Int*., in press (2019). https://doi.org/10.1029/2018JB016778
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198. H. Yang, J.-F. Lin, M. Y. Hu, M. Roskosz, W. Bi, J Zhao, E. E. Alp, J. Liu, T. Okuchi, R. M. Wentzcovitch, and N. Dauphas, **Iron isotope fractionation in Earth's lower mantle mineral phases: did terrestrial magma ocean crystallization fractionate iron isotopes?**, *Earth and Planet. Sc. Lett.* **516**, 113-122 (2019). DOI:10.1016/j.epsl.2018.10.034

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166. Z. Wu and R. Wentzcovitch, **Spin crossover in ferropericlase and lateral heterogeneities in the Earth's lower mantle**, *Proc. Nat. Acad. Sc. USA* **111**, 10468-10472 (2014). DOI: 10.1073/pnas.1322427111

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162. S. Q. Wu, M. Ji, C. Z. Wang, M. C. Nguye, X. Zhao, K. Umemoto, R. M. Wentzcovitch, and K. M. Ho, **Adaptive genetic algorithm for crystal structure prediction**, *J. Phys.: Cond. Matter* **26**, 035402 (2014). DOI:10.1088/0953-8984/26/3/035402

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158. M. Núñez-Valdéz, Z. Wu, Y. Yu, and R. M. Wentzcovitch, **Thermal elasticity of $(Fe_x,Mg_{1-x})_2SiO_4$ olivine and wadsleyite,** *Geophys. Res. Lett.* **40**, 290–294 (2013), DOI:10.1002/grl.50131.

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157. T. Sun and R. Wentzcovitch, **Direct Determination of Electric Current in Born-Oppenheimer Molecular Dynamics**, *Chem. Phys. Lett.* **554**, 15-19 (2012). (*Editor's choice*) DOI: 10.1016/j.cplett.2012.10.052

156. R. M. Wentzcovitch, H. Hsu, and K. Umemoto, **Spin state crossovers in iron bearing perovskite: a review of first principles studies**, *Europ. J. Mineral*. *(special issue)* **24**, 851-862 (2012). DOI: 10.1127/0935-1221/2012/0024-2249

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154. M. Núñez-Valdéz, Z. Wu, Y. Yu, J. Revenaugh, and R. M. Wentzcovitch, **Thermoelastic properties of wadsleyite and ringwoodite $(Fe_x,Mg_{1-x})_2SiO_4$: their relationship to the 520 km seismic discontinuity**, *Earth & Planet. Sc. Lett.* **351-352**, 115-122 (2012). DOI: 10.1016/j.epsl.2012.07.024

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5. R.M. Wentzcovitch, M. Cardona, M.L. Cohen, and N. Christensen, **X_1 and X_3 states of electrons and phonons in zincblende semiconductors**, *Sol. Stat. Comm.* **67**, 927 (1988).

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3. CONFERENCE PUBLICATIONS

C18. P. da Silveira, A. Holiday, M. Núñez-Valdéz, L. Gunathilake, D. A. Yuen, and R. M. Wentzcovitch, **First principles elasticity workflow in the *Vlab* Science Gateway**, *Proc. of XSEDE'13 Conference* (2013).
http://vlab.msi.umn.edu/reports/proposal/papers/S6-VLab_Ab_initio-xsede13.pdf

C17. P. da Silveira, M. Núñez-Valdéz, R. M. Wentzcovitch, M. Pierce, and D. A. Yuen, **VLab: an updated overview of system service and architecture**, *Proc. of Teragrid 2011 Conference*, http://dl.acm.org/citation.cfm?doid=2016741.2016777 (2011).

C16. C. R. S. da Silva, P. Da Silveira, B. B. Karki, R. M. Wentzcovitch, **VLab: a cyberinfrastructure for parameter sampling computations in Materials Science**, *IEEE International Symposium on ClusterComputing and the Grid—CCGrid 2007*, Rio de Janeiro—Brazil, May 14-17, (2007).

C15. R. M. Wentzcovitch, **Spin transition in magnesiowustite in Earth's lower mantle,** *Geochimica et Cosmochimica Acta* , **71**, 3772 (2007).

C14. K. Umemoto, R. M. Wentzcovitch, L. Wang, and C. Leighton, **Electronic structure of $Co_{1-x}Fe_xS_2$,** *Phys. Stat. Sol. (b)*, **243**, 2117 (2006). DOI: 10.1002/pssb.200666821

C13. T. Tsuchiya, R. M. Wentzcovitch, C. R. da Silva, S. de Gironcoli, J. Tsuchiya, **Pressure induced high spin to low spin transition in magnesiowüstite,** *Phys. Stat. Sol. (b)*, **243**, 2111 (2006). DOI: 10.1002/pssb.200666814

C12. J. R. Chelikowsky, T. Kaxiras, and R. M. Wentzcovitch, **Theory of spintronic materials**, *Phys. Stat. Sol. (b)*, **243**, 2133 (2006). DOI: 10.1002/pssb.200666817

C11. R. M. Wentzcovitch, **Similarities and contrasts in pressure induced amorphization: insights from first principles studies**, Proceedings of CECAM Workshop on Atomic structure and transport in glassy networks (2002).

C10. L. P. Stixrude, R. M. Wentzcovitch, B. Kiefer, and C. R. S. da Silva, **Ab Initio Investigation of the High Pressure Elasticity of Mg_2SiO_4 Forsterite and Ringwoodite**, *MRS Proceedings* **499**, 15 (1998).

C9. W. Duan, G. Paiva, R. Wentzcovitch, and A. Fazzio, **Ruby's optical transitions: effects of pressure induced phase transformation**, *MRS Proceedings* **499**, 275 (1998).

C8. J. R. Chelikowsky, R. M. Wentzcovitch, C. R. S. da Silva, and N. Binggeli, **A new pressure induced phase in silica**, *MRS Proceedings*, **499**, 243 (1998).

C7. R. S. da Silva and R. M. Wentzcovitch, **A phenomenological equation of state for the lower mantle**, Proceedings of CECAM Workshop on How can *ab initio* calculations contribute to mineral physics, Lyon, France (1997).

C6. R. M. Wentzcovitch. C. R. S. da Silva, J. R. Chelikowsky, and N. Binggeli, **New phase and gradual coordination change in silica under pressure**, Proceedings Adriatico Research Conference on Simple systems at high pressures and temperatures: theory and experiment, Trieste, Italy (1997).

C5. K. T. Thomson, W. Duan, and R. M. Wentzcovitch, **Polymorphs of alumina predicted by first principles: implications for the ruby high pressure scale**, Proceedings of Conf. on High Temperature Materials, Santa Fé, USA (1997).

C4. R. M. Wentzcovitch, G. D. Price, and N. L. Ross, ***Ab initio* constant pressure molecular dynamics study of silicated perovskites**, Mineralogical Magazine, **58A**, 963 (1994) (ISSN 0026-461X). Proceedings of the VM Goldschmidt Conference, Edinburgh, UK (1994).

C3. J. H. Kim, K. Levin, R. M. Wentzcovitch, and A. Auerbach, **The effect of strong Coulomb correlations on electron-phonon interactions in the copper oxides: Implications for transport**, Proceedings of Conf. on Electron-phonon interactions in Copper Oxides, (Mexico) (1991).

C2. R. M. Wentzcovitch, A. Continenza, and A. J. Freeman, **The role of polarity on the stability of graphitic compounds**, *Diamond, silicon* carbide *and related wide bandgap semiconductors, MRS Proceedings* **162**, 611 (1990).

C1. A.L. Liu, R. M. Wentzcovitch, and M. L. Cohen, **Atomic arrangement and electronic structure of BC_2N**, in *Graphite and Graphite Intercalation Compounds*, Symposium L of the Fall meeting of the Materials Research Society, ed. by M. Endo, M. S. Dresselhaus, and G. Dresselhaus (1988).

4. VIDEO

V1. C. R. S. da Silva and R. M. Wentzcovitch, **First principles investigation of the A7 to simple cubic transformation in As**, *Comp. Mat. Sci.'s* video library, (accompanied by an article, Ref. 45).

H. INVITED PRESENTATIONS

Renata Wentzcovitch and members of her group have presented ~270+ invited talks and seminars. They consistently present 20+ contributed talks/posters per year in APS, AGU, COMPRES, and other meetings.

Conferences and Workshops

118 **"Post-PPV transitions in $MgSiO_3$ in Super-Earth's mantles"**, American Chemical Society 2019 Meeting, Orlando, USA (*04/19*).

117 **"Spin Crossover in Iron in Lower Mantle Minerals"**, American Physical Society 2019 March Meeting, Boston, USA (*03/19*).

116 **"Spin Crossover in Iron in Lower Mantle Minerals"**, Materials and Molecular Modeling Hub Conference 2018, Thomas Young Centre, The London Centre for the Theory and Simulation of Materials, London, UK (*08/18*).

115 **"Spin Crossover in Iron in Lower Mantle Minerals"**, International Conference in Computational Physics, Davis, USA (*07/18*).

114 **"Spin Crossover in Iron in Lower Mantle Minerals and some Geophysical Consequences"**, International Workshop on Geodynamics and Big Data, Sardinia, Italy (*06/18*).

113 **"Spin Crossover in Iron in Lower Mantle Minerals and some Geophysical Consequences"**, Workshop on Practical Quantum Mechanics for Electronic Materials, Austin, USA (*06/18*).

112 **"A Hell of a Problem (or a Problem from Hell): Spin Crossover in Iron in the Deep Earth"**, ES'17: Recent Developments in Electronic Structure Theory, Princeton, USA (*06/17*).

111 **"New Trends and Recent Achievements in Theoretical High Pressure Research"**, **Plenary Talk**, 54th International Meeting of European High Pressure Group (EHPRG), Bayreuth, Germany (*09/16*).

110 **"Nature of the Volume Isotope Effect in Ice"**, 17th International Conference on High Pressure Semiconductor Physics (HPSP-17), Tokyo, Japan (*08/16*).

109 **"Spin crossover in ferropericlase and lateral velocity variations in the Earth's mantle",** High Pressure Gordon Research Conference, Holderness, NH, USA (*07/16*).

108 **"Spin crossover in mantle minerals: some geophysical consequences"**, Workshop on **"**Next Generation Quantum Materials**"**, International Center for Theoretical Physics – South American Institute for Fundamental Research (ICTP-SAIFR), São Paulo, SP, Brazil (*04/16*).

107 **"Spin crossover in mantle minerals"**, 2015 IUCr High-Pressure Workshop, Campinas, SP, Brazil (*09/15*).

106 **"Spin crossover in ferropericlase and lateral velocity variations in the Earth's mantle"**, Joint AIRAPT-EHPRG'2015 Conference, Madrid, Spain (*09/15*).

105 **"Spin crossover in ferropericlase and lateral velocity variations in the Earth's mantle"**, **Key-Note Lecture,** Symposium 25d: Physics and Chemistry of Earth Materials, Goldschmidt Conference, 25th Anniversary, Prague, Czeck Republic (*08/15*).

104 **"Spin crossover in (Mg,Fe)O"**, Symposium 4A: Advances in Computational Materials Science, XXIV International Materials Research Congress – Cancun, Mexico, (*08/15*).

103 **"Spin crossover in (Mg,Fe)O and implications for Earth's internal structure"**, Brazilian Physical Society Meeting, Foz do Iguaçu, Brazil *(05/15)*.

102 **"Spin crossover in ferropericlase and lateral heterogeneities in the lower mantle"**, International Conference in Semiconductor Physics, Austin, USA *(07/14)*.

101 **"Elastic Anomalies in a Spin-Crossover System: Ferropericlase at Lower Mantle Conditions"**, International Conference in Semiconductor Physics, Austin, USA *(07/14)*.

100 **"Phonon gas model workflow in the *VLab* Science Gateway",** American Geophysical Union Fall 2013 Meting, San Francisco, USA (*12/13*).

099 **"Anharmonic effects and heat transport in complex systems",** American Geophysical Union Fall 2013 Meting, San Francisco, USA (*12/13*).

098 **"*VLab*: a Science Gateway for computational mineral physics",** COMPRES/DEFORM NSF EarthCube Workshop, Alexandria, VA, USA *(11/13)*.

097 **"The *VLab* Science Gateway for Computational Mineral Physics",** Planning Workshop for the NSF Science Gateway Institute, Baltimore, USA *(03/13)*.

096 **"Recent advances in computational mineral physics"**, Materials Genome Project Workshop on Thermodynamics Databases for Geochemical Applications, Miami, USA *(03/13)*.

095 **"Interactive database of thermodynamics properties of minerals in the *VLab* Science Gateway",** EarthCube Workshop, Smithsonian Institution, Washington DC, USA *(03/13)*.

094 **"Spin state crossovers in mantle minerals"**, International Symposium Nanoscience and Quantum Physics 2012, nanoPHYS'12, Tokyo, Japan (*12/12*).

093 **"Elasticity of ferropericlase at lower mantle conditions"**, American Geophysical Union Fall 2012 Meting, San Francisco, USA (*12/12*).

092 **"Post-stishovite transition in hydrous SiO_2",** American Geophysical Union Fall 2012 Meting, San Francisco, USA (*12/12*).

091 **"*VLab*: a Science Gateway for computational mineral physics",** EarthScope, NSF EarthCube Workshop, Arizona State University, Tempe, USA *(10/12)*.

090 **"The role of first principles calculations in mineral physics**, Frontiers in Geosciences Conference, University of São Paulo , São Paulo, Brazil (07/12).

089 **"Spin state crossovers in lower mantle minerals"**, 24th Annual Workshop on Recent Developments in Electronic Structure Theory (ES2012), Winston-Salem, USA (06/12).

088 **"Modeling the Earth from atomic to global Scale"**, Public Lecture at *AIC Boys Secondary School*, in conjunction with the African School Series on Electronic Structure Methods and Applications (**ASESMA**), Eldoret, Kenya (*05/12*).

087 **"Modeling the Earth from atomic to global Scale"**, Public Lecture at the African School Series on Electronic Structure Methods and Applications (**ASESMA**), Chepkoilel University College, School of Science, Eldoret, Kenya (*05/12*).

086 **"Spin state crossovers in lower mantle minerals in and in $LaCoO_3$: a common perspective"**, African School Series on Electronic Structure Methods and Applications (**ASESMA**), Eldoret, Kenya (*05/12*).

085 **"Thermodynamics and thermoelastic properties of minerals: the ingredients of geophysical modeling"**, **"**USC-DOE: Materials Genome Conference**"**, Ranchos Palos Verdes, CA, *USA (04/12).*

084 **"Spin state crossovers in lower mantle minerals"**, Spring ACS Meeting Symposium **"**Quantum Chemistry for Geochemistry**"**, San Diego, USA *(03/12).*

083 **"Spin state crossovers in mantle minerals"**, Workshop on Formation of Novel Phases under Extreme Condition, Los Alamos, USA (*12/11*).

082 **"Spin state crossovers in mantle minerals"**, American Geophysical Union Fall 2011 Meting, San Francisco, USA (*12/11*).

081 **"Spin state crossovers in mantle minerals"**, 7th European Conference on Mineralogy and Spectroscopy, Potsdam, Germany (*09/11*).

080 **"Spin state crossovers in mantle minerals"**, Elizabeth and Frederick White Conference on **"**Minerals at Extreme Conditions: Integrating Theory and Experiments**"**, Australia Academy of Sciences, Canberra, Australia (*04/11*).

079 **"Spin state crossovers in mantle minerals"**, APS March Meeting, Dallas, USA, (*03/11*)

078 **"Spin state crossovers in mantle minerals"**, CECAM Workshop: Computational Mineral Physics: Applications to Geophysics, Zurich, Switzerland (*10/10*).

077 **"Spin crossovers in mantle minerals in spintronic materials"**, Psi-K 2010, Berlin, Germany (*09/10*).

076 **"First principles research on deep Earth's materials"**, African School of Electronic Structure Methods and Applications (ASESMA), Cape Town, South Africa (*07/10*).

075 **"The Quasiharmonic Approximation - QHA"**, African School of Electronic Structure Methods and Applications (ASESMA), Cape Town, South Africa (*07/10*).

074 **"Silica"**, African School of Electronic Structure Methods and Applications (ASESMA), Cape Town, South Africa (*07/10*).

073 **"Spin-state crossover of iron in lower mantle minerals: results of DFT+U investigations"**, MSA Short Course: Theoretical and Computational Methods in Mineral Physics: Geophysical Applications, Berkeley, USA (*12/09*).

072 **"Thermoelasticity properties of minerals using first principles quasiharmonic theory"**, MSA Short Course: Theoretical and Computational Methods in Mineral Physics: Geophysical Applications, Berkeley, USA (*12/09*).

071 **"Thermoelastic properties of ferropericlase across its spin transition in the lower mantle"**, AGU Joint Assembly – Meeting of the Americas, Toronto, Canada (*05/09*).

070 **"Exploring mantle mineralogy of terrestrial exoplanets"**, National Ignition Facility, Liveremore (LLNL), USA (*12/08*).

069 **"Thermoelastic properties of ferropericlase across its spin transition in the lower mantle"**, American Geophysical Union, Fall08 AGU Meeting, San Francisco, USA (*12/08*).

068 **"Spin Crossover Transitions in lower mantle minerals"**, Computational Science Workshop'09, Tsukuba, Japan (*12/08*).

067 **"Thermoelastic properties of ferropericlase across its spin transition in the lower mantle"**, Onsen Workshop on **"**Transport Properties in the Mantle**"**, Yunishigawa, Japan (*10/08*).

066 **"First principles quasiharmonic calculations of Earth minerals and applications to the Earth's mantle"**, CECAM Workshop on Minerals Spectroscopy: from Experiments and Theory, Lausanne, Switzerland, *(10/08)*

065 **"First principles thermoelasticity of Earth minerals"**, ThermodynaMix II Workshop, Barcelona, Spain *(10/08)*.

064 **"Elasticity of ferropericlase across the spin transition"**, Workshop on Pseudopotential Methods in Electronic Structure: James R. Chelikowsky Festschrift, TX, USA *(04/08)*.

063 **"P-V-T relations in MgO: an ultrahigh pressure scale for planetary sciences applications"**, American Geophysical Union, Fall07 AGU Meeting, San Francisco, USA (*12/07*).

062 **"Elasticity of ferropericlase across the spin transition"**, American Geophysical Union, Fall07 Meeting, San Francisco, USA (*12/07*).

061 **"Elasticity of ferropericlase across the spin transition"**, 2nd ***VLab*** Workshop, Minneapolis, USA (*08/07*).

060 **"Spin transition in magnesiowüstite and consequences for elasticity"**, Goldshmidt Conference 2007, (keynote lecture) Köln, Germany (*08/07*).

059 **"Theory of Materials at Ultrahigh Pressures and Temperatures: the Coming of Age of Planetary Materials Science"**, Workshop on Novel Methods in Electronic Structure, Institute for Mathematics and its Applications, Minneapolis, Minneapolis, USA (*08/07*).

058 **"Spin transition in magnesiowüstite and consequences for elasticity"**, The 16th International Symposium on the reactivity of solids, Minneapolis, USA (*06/07*).

057 **"Theory of materials at ultrahigh pressures and temperatures: the coming of age of planetary materials science"**, EuroMinSci Conference (keynote talk), Nice, France (*03/07*).

056 **"P-V-T relations in MgO: an ultrahigh pressure scale for planetary sciences applications"**, Workshop on **"**High Pressure Scales**"**, Carnegie Institution of Washington, Washington D.C., USA (*01/07*).

055 **“Theory of Materials at Ultrahigh Pressures and Temperatures: the Coming of Age of Planetary Materials Science”**, American Chemical Society, San Francisco, USA (*09/06*).

054 **“Minerals at Condition of the Giant’s Interiors”**, General Meeting of the International Mineralogical Association, Kobe, Japan *(07/06*).

053 **“Spin Transition in Iron Doped Minerals Under Pressure”**, American Ceramics Society, Spring 2006, Baltimore *(05/06*).

052 **“Spin Transition in Magnesiowüstite Under Pressure”**, Workshop on Synergy of 21st Century High-Pressure Science and Technology, Argonne National Laboratory, USA, (*04-05/06*).

051 **“Spin Transition in Magnesiowüstite Under Pressure: Elastic Properties”**, American Geophysical Union, Fall05 Meeting, San Francisco, USA (*12/05*).

050 **“Spin Transition in Magnesiowüstite Under Pressure”**, Workshop on Computational Materials and Molecular Electronics, Austin, USA (*10/05*).

049 **“MgSiO3 Post-perovskite at D” Conditions”,** International Workshop on the Post-Perovskite Phase Transition in the Earth’s Deep Mantle, Tokyo, Japan *(10/05).*

048 **“MgSiO3 Post-perovskite at D” Conditions”,** Earth's Mantle Composition, Structure, and Phase Transitions, Saint-Malo, France *(08/05).*

047 **“MgSiO3 Post-perovskite at D” Conditions”,** 1st ***Vlab*** Workshop, 2005, Minneapolis, USA *(07/05).*

046 **“The Role of First Principles Calculations in Geophysics”,** Symposium in honor of Marvin Cohen's 70th Birthday, Berkeley, USA (*03/05*).

045 **“Post-perovskite Transition in MgSiO3”,** European High Pressure Research Group Annual Meeting (EHPRG ’42), Lausanne, Switzerland (*09/04*).

044 **“Phase Transition in $MgSiO_3$ Perovskite in Earth’s Lower Mantle”,** CIDER Workshop, Kavli Institute for Theoretical Physics, UC-Santa Barbara, Santa Barbara, USA (*07/04*).

043 **“Post-perovskite Transition in MgSiO3”,** COMPRES Annual Meeting, Reno, USA *(6/04).*

042 **“Thermoelastic Properties of Post-perovskite MgSiO3”,** Elasticity Grand Challenge COMRES Meeting, Urbana Champaign, USA *(05/04).*

041 **“Thermoelastic Properties of Post-perovskite MgSiO3”,** Joint Assembly AGU, CGU, SEG, EEGS, Montreal, Canada *(05/04).*

040 **"Thermoelasticity of $MgSiO_3$-perovskite: Consequences for the Inferred Properties of the Lower Mantle"**, Annual Meeting of the German Mineralogical Society (DMG) *(plenary talk),* Bochun, Germany (*09/03*).

039 **“Quasiharmonic Thermal Properties of Minerals”,** 15th Annual Workshop on Recent Developments in Electronic Structure Methods (Electronic Structure'03), Minneapolis, USA (*05/03*).

038 **"Thermoelasticity of $MgSiO_3$-perovskite at Lower Mantle Conditions"**, Joint Congress of the American Geophysics Union, European Geophysical Society, and European Geophysical Union, Nice, France (*04/03*).

037 **"Thermoelasticity of $MgSiO_3$-perovskite at Lower Mantle Conditions"**, 2nd Workshop on Mantle Composition, Structure and Phase Transitions, Frejus, France (*04/03*).

036 **"Theory of Materials at High Pressures and Temperatures",** NSF-COMPRES workshop, Miami, USA (*03/03*).

035 **"Thermoelasticity of $MgSiO_3$-perovskite: Consequences for the Inferred Properties of the Lower Mantle"**, XI International Workshop on Computational Materials Science: Total Energy and Force Methods" at the ICTP, Trieste, Italy (*01/03*).

034 **"Thermoelasticity of $MgSiO_3$-perovskite at Lower Mantle Conditions"**, American Geophysics Union, San Francisco, USA (*12/02*).

033 **"Contrasts and Similarities in Pressure Induced Amorphization",** CECAM workshop on **"**Atomic Structure and Transport in Glassy Networks**"**, Lyon, France (*06/02*).

032 **"Thermoelasticity of $MgSiO_3$-perovskite at Lower Mantle Conditions"**, Materials Research Society, Spring'02, Symposium on **"**Perovskite Materials**"**, San Francisco, USA (*04/02*).

031 **"Optical and Structural Transitions in Ruby: A Tale of Two Oxides",** CECAM workshop on **"**Electronic Properties of Strongly Correlated Systems: from the Local Density Approximation to the Dynamical Mean Field Theory**"**, Lyon, France (*7/01*).

030 **"Optical and Structural Transitions in Ruby: A Tale of Two Oxides"**, CECAM workshop on **"**Stress-driven Solid-solid Transformation**"**, Lyon, France (*07/01*).

029 **"Thermoelasticity of Minerals by First Principles"**, CECAM workshop on **"***Ab Initio* Calculations in Geophysics**"**, Lyon, France (*07/01*).

028 **"High Pressure and the Earth Mantle"**, workshop on **"**Future Directions in High Pressure Research**"**, organized by Ike Silvera and Bill Nellis, San Francisco, USA (*03/01*).

027 **"First principles thermoelasticity of mantle minerals"**, **"**Mardi Gras Conference on Multiscale Simulation, Theoretical and Experimental Approaches to Deformation, Fatigue, and Fracture**"**, Baton Rouge, USA (*02/01*).

026 **"First Principles Molecular Dynamics"**, Lecture series at the Pan-American Advanced Studies Institute in Computational Materials Science, Santiago, Chile, sponsored by NSF, DOE, and UNESCO (*01/01*).

025 **"First Principles Thermoelasticity of Minerals"**, Gordon Research Conference on Research at High Pressures, New Hampshire. USA (*06/00*).

024 **"First Principles Thermoelasticity of Minerals: Geophysical Implications"**, International Conference on Multiscale Materials Phenomena in Harsh Environments, Limassol, Cyprus (*06/00*).

023 **"First Principles Thermoelasticity of Minerals: Geophysical Implications"**, APS Satellite Meeting. **"**Fifteen Years of the Car-Parrinello Method in Physics and Chemistry**"**, Minneapolis, USA (*03/00*).

022 **"Thermoelasticity of Minerals from First Principles"**, CECAM Workshop on Frontiers in High Pressure Physics, Lyon, France (*07/99*).

021 **"Optical Transitions in Ruby Across the Corundum to Rh_2O_3(II) Transformation"**, International Conference on High Pressure Science and Technology, AIRAPT, Honolulu, USA (*07/99*).

020 **"Optical Transitions in Ruby across the Corundum to Rh_2O_3(II) Transformation"**, 5th International Conference in Advanced Materials, International Union of Materials Research Societies, Beijing, China (*06/99*).

019 **"Elasticity of Minerals from First Principles"**, APS Centennial Meeting, Atlanta, USA (*03/99*).

018 **"Silica and Alumina: New Discoveries in Old Systems"**, UC-Davis Materials Research Institute Workshop on Electronic Structure, Davis, USA (*03/98*).

017 **"New Phase and Gradual Coordination Change in Silica Under Pressure"**, American Geophysical Union, San Francisco, USA (*12/97*).

016 **"New Phase and Gradual Coordination Change in Silica Under Pressure"**, Materials Research Society, Fall'97, with J. R. Chelikowsky, C. R. S. da Silva, and N. Binggeli, Symposium on **"**High Pressure Materials Research**"** (*11/97*).

015 **"First Principles Investigation of Elasticity of Earth Materials Under Pressure"**, with L. Stixrude (speaker), B. Kiefer, and C. R. S. da Silva, Materials Research Society, Fall'97, Symposium on **"**High Pressure Materials Research**"**, (*11/97*).

014 **"New Phase and Gradual Coordination Change in Silica Under Pressure"**, Mardis Gras Conference on **"**Materials Under Extreme Conditions**"**, Baton Rouge, USA (*02/97*).

013 **"New Phase and Gradual Coordination Change in Silica Under Pressure"**, Workshop on **"**Computer-Aided Design of High Temperature Materials, Santa Fé, USA (*08/97*).

012 **"New Phase and Gradual Coordination Change in Silica Under Pressure"**, Adriatico Research Conference on **"**High Pressure Materials Research: Theory and Experiment**"**, Trieste, Italy (*07/97*).

011 **"New Phase and Gradual Coordination Change in Silica Under Pressure"**, CECAM Workshop on Mineral Physics, Lyon, France (*06/97*).

010 **"Pressure Induced Amorphization in BAs: a Possible Inhibited Dissociation"**, Electronic Structure'96, Minneapolis (*06/96*).

009 ***"Ab initio Study* of Mantle Minerals at Lower Mantle Pressures"**, with G. D. Price (speaker) and N. Ross, VM Goldschmidt Conference, Edinburgh, UK (*09/94*).

008 ***"Ab initio* Molecular Dynamics with Variable Cell Shape"**, Gordon Research Conference on Structural Phase Transitions, Volterra, Italy (*05/94*).

007 **"Ab initio Molecular Dynamics with Variable Cell Shape: Application to $MgSiO_3$-perovskite"**, American Geophysical Union. San Francisco (*12/93*).

006 ***"Ab initio* Study of Mantle Minerals at Lower Mantle Pressures"**, London-Oxford-Cambridge Mineral Physics Symposium, Oxford, UK (*11/93*).

005 ***"Ab initio* Molecular Dynamics with Variable Cell Shape"**, Swiss/Italian Workshop on Electronic Structure and Parallel Calculation, Cagliari, Italy (*08/93*).

004 ***"Ab initio* Molecular Dynamics with Variable Cell Shape"**, Brazilian Physical Society, Condensed Matter Division, Caxambu, Brazil (*05/93*).

003 ***"Ab initio* Molecular Dynamics with Variable Cell Shape"**, APS March Meeting, Seattle USA (*3/93*).

002 ***"Ab initio* Molecular Dynamics with Variable Cell Shape: Application to $MgSiO_3$-perovskite"**, London-Oxford-Cambridge Mineral Physics Symposium, London, UK (*11/92*).

001 ***"Ab initio* Molecular Dynamics with Variable Cell Shape",** Fourth Annual Workshop on Recent Developments in Electronic Structure Methods (Electronic Structure'92), Raleigh. USA (*05/92*).

Department Seminars/Colloquia

93. **"Spin Crossover in Iron in Lower Mantle Minerals"**, Department of Physics, Stony Brook University, Stony Brook, USA (*10/18*).

92. **"Ab initio simulations of planetary materials"**, Department of Applied Physics and Applied Mathematics, APAM Research Conference Series, Columbia University, New York, USA (*10/17*).

91. **"Spin Crossover in Iron in the Deep Earth"**, Department of Earth Sciences, Princeton, USA (*10/17*).

90. "**Spin Crossover in Iron in Lower Mantle Minerals",** Lamont Doherty Earth Observatory, "Hot Topics" Seminar Series (*04/17*).

89. "**Spin Crossover Systems in the Deep Earth",** Department of Physics, Tsinghua University (*11/16*).

88. "**Nature of the Volume Isotope Effect in Ice",** Department of Geology, University of Frankfurt (*11/16*).

87. "**Spin Crossover in Iron Bearing Minerals",** Center for Functional Materials, Brookhaven National Laboratory (*12/15*).

86. "**Spin Crossover in Iron Bearing Minerals",** Center for Functional Materials, Brookhaven National Laboratory (*12/15*).

85. "**Modeling Earth Interior from Atomic to Global Scale"**, Department of Geosciences, Stony Brook University (*12/15*).

84. "**Modeling Earth Interior from Atomic to Global Scale"**, Institute for Advanced Computational Science, Stony Brook University (*12/15*).

83. "**The role of *Ab initio* Calculations in Geophysics"**, Lamont Doherty Earth Observatory, Columbia University (*11/15*).

82. "**Modeling Earth Interior from Atomic to Global Scale"**, Department of Applied Physics and Applied Mathematics, Columbia University (*11/15*).

81. "**Spin Crossover in ferropericlase and lateral heterogeneities in Earth's lower mantle"**, Physics Department Colloquium, University of Toronto, Toronto, Canada (*10/15*).

80. "**Modeling Earth Interior from Atomic to Global Scale"**, Computational Science Research Center, Chinese Academy of Engineering Physics, Beijing, China (*06/15*).

79. "**Spin Crossover in ferropericlase and lateral variations in Earth's lower mantle"**, Physics Department, Tokyo-Tech, Tokyo, Japan (*01/15*).

78. "**Spin Crossover in ferropericlase and lateral variations in Earth's lower mantle"**, Earth and Life Sciences Institute, Tokyo-Tech, Tokyo, Japan (*08/14*)

77. **"Modeling Earth from atomic to global scale",** Regional Council of Engineering and Agronomy of Rio de Janeiro (CREA), Geology and Mines Chamber, Rio de Janeiro, RJ, Brazil *(05/14).*

76. **"Modeling Earth from atomic to global scale",** Department of Physics, Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil *(05/14).*

75. **"Modeling Earth from atomic to global scale",** Department of Physics, Federal University of ABC, Santo André, SP, Brazil *(07/13).*

74. **"Modeling Earth from atomic to global scale",** Department of Physics, Tokyo Institute of Technology, Tokyo, Japan, *(12/12).*

73. **"The role of first principles calculations in Geophysics"**, School of Earth and Space Science, University of Science and Technology of China, Hefei, China *(07/12)* .

72. **"Spin crossover systems in the Earth lower mantle"** , Department of Physics, University of Science and Technology of China, Hefei, China *(07/12)* .

71. **"The role of first principles calculations in mineral physics"**, Department of Geology, U. of Frankfurt, Goethe University, Frankfurt, Germany (*05/12*).

70. **"Spin state crossovers in mantle minerals"**, Department of Physics, Auburn University, Auburn, USA (*02/12*).

69. **"Spin state crossovers in mantle minerals"**, Magnetics Seminar, Department of Electrical Engineering, U. of Minnesota, Minnepolis, USA (*12/11*).

68. "**Spin crossovers in mantle minerals and in spintronic materials"**, Interactive Research Center of Science, Tokyo Institute of Technology, Tokyo, Japan. (*07/10*).

67. "**Spin crossover systems in Earth's lower mantle and in Leighton's Lab**", Department of Earth and Planetary Sciences, Tokyo Institute of Technology, Tokyo, Japan (*05/10*).

66. "**First principles quasiharmonic thermoelastic properties of minerals**", Department of Aerospace and Mechanical Engineering, U of Minnesota, Minneapolis, USA (*04/10*).

65. "**Spin crossover systems in Earth's lower mantle and in Leighton's Lab**", Department of Chemical Engineering and Materials Science, U of Minnesota, Minneapolis, USA (*04/10*).

64. "**Advances and challenges in the theory of planetary materials**", NCSA Director's Seminar, University of Illinois, Urbana-Champaign, USA (*12/09*).

63. "**Thermoelastic properties of minerals using first principles quasiharmonic theory**", Minnesota Supercomputing Institute, Scientific Computation Seminar Series, U. of Minnesota, Minneapolis, USA (*10/09*).

62. "**First principles thermodynamics of mantle minerals"**, Department of Chemical Engineering, University of Bologna, Bologna, Italy (*09/09*).

61. "**Spin crossover transition in ferropericlase in Earth's mantle**", Department of Geosciences, Virginia Tech, Blacksburg, USA (*04/09*).

60. "**Advances and challenges in theory of planetary materials**", Department of Geophysics Chinese Academy of Sciences, Beijing, China (*03/09*).

59. "**Advances and challenges in the theory of Earth and Planetary Materials**", Department of Physics, Tsinghua University, Beijing, China (*03/09*).

58. "**Spin Crossover transition in ferropericlase in Earth's mantle**", Department of Physics, Tsinghua University, Beijing, China (*03/09*).

57. "**Spin Crossover transition in ferropericlase in Earth's mantle**", Hawai'i Institute of Geophysics and Planetology, University of Hawai'i, Honolulu, USA (*02/09*).

56. "**Spin Crossover transition in ferropericlase in Earth's mantle**", Department of Physics, University of Alberta, Edmonton, Canada (*01/09*).

55. "**Thermoelastic properties of ferropericlase**", Department of Earth and Planetary Sciences, Tokyo Institute of Technology, Tokyo, Japan (*11/08*).

54. "**Thermoelastic properties of ferropericlase**", Department of Geological Sciences, Tohoku University, Sendai, Japan (*11/08*).

53. "**Advances and challenges in theory of planetary materials",** Department of Applied Physics, University of Tokyo (Todai-mae), Japan (*11/08*).

52. "**Advances and challenges in theory of high pressure materials**", Institute for Solid State Physics (ISSP), University of Tokyo, Japan, (*11/08*).

51. **"The role of first principles calculations in geophysics"**, Instituto Nazionale the Geofisica e Vulcanologia, Rome, Italy, *(10/08)*.

50. "**Advances and Challenges in the Theory of Planetary Materials**", Department of Chemical and Materials Engineering, University of Alberta, Edmonton, Canada, *(09/08)*.

49. **"Elasticity of ferropericlase across the spin transition"**, Department of Physics and Astronomy, Stony Brook University, Stony Brook, USA (*08/08*).

48. **"Elasticity of ferropericlase across the spin transition"**, Department of Electrical Engineering, U. Minnesota, Minneapolis, USA (*10/07*).

47. "**Invariant Molecular Dynamics Approach to Structural Phase Transition**", Department of Physics, Tokyo Institute of Technology, Tokyo, Japan (*07/06*).

46. "**Advances and Challenges in the Theory of Planetary Materials**", Department of Physics, Tokyo Institute of Technology, Tokyo, Japan (*07/06*).

45. "**Spin transition in Magnesiowustite in Earth's mantle**", Department of Earth and Planetary Sciences, Tokyo Institute of Technology, Tokyo, Japan (*07/06*).

44. **"Advances and Challenges in the Theory of Planetary Materials**", Seminar at the Department of Physics, University of Nevada, Las Vegas, USA (*03/06*).

43. "**Advances and Challenges in the Theory of Planetary Materials**", Colloquium at the Department of Physics and Astronomy, University of Minnesota, Minneapolis, USA (*02/06*).

42. "**Advances and Challenges in the Theory of Planetary Materials**", Colloquium at the Department of Physics and Astronomy, Stony Brook University, Stony Brook, USA (*11/05*).

41. "**Spin transition in Iron Doped Minerals**", Institute for the Theory of Advanced Material in Information Technology, U. of Minnesota, Minneapolis , USA (*07/05*).

40. **"$MgSiO_3$ Post-Perovskite at D" Conditions**", Department of Earth, Atmospheric, and Planetary Sciences, MIT, Boston (*04/05*).

39. **"$MgSiO_3$ Post-Perovskite at D" Conditions**", SUNY-Stony Brook, Department of Geosciences, SUNY-Stony Brook, Stony Brook, USA (*01/05*).

38. **"$MgSiO_3$ Post-Perovskite at D" Conditions**", Department of Geosciences, University of Chicago, Chicago, USA (*01/05*).

37. **"Phase Transition in $MgSiO_3$ Perovskite in Earth's Lower Mantle**", DEMOCRITOS National Simulation Center, SISSA, Trieste, Italy (*08/04*).

36. **"Composition Controlled Spin Polarization in Co1-xFexS2",** Institute for the Theory of Advanced Material in Information Technology, U. of Minnesota, Minneapolis , USA (*07/04*).

35. **"Thermoelasticity of $MgSiO_3$-perovskite: Consequences for the Inferred Properties of the Lower Mantle"**, Seismology Laboratory, Harvard University, Boston, USA (*11/02*).

34. **“Thermoelastic Properties of Lower Mantle Minerals”,** Umbgrove Lecture, Faculty of Geosciences, University of Utrecht, Holland *(05/04).*

33. **"Thermoelasticity of $MgSiO_3$-perovskite: Consequences for the Inferred Properties of the Lower Mantle"**, Department of Earth and Planetary Sciences, Washington University, Saint Louis, USA (*11/02*).

32. **"Thermoelasticity of Minerals from First Principles"**, Department of Geology, University of Illinois, Urbana-Champaign, USA (*11/02*).

31. **"Thermoelasticity of Minerals from First Principles"**, Department of Physics, Ohio State University, Columbus, USA (*10/02*).

30. **"Thermoelasticity of Minerals from First Principles"**, Department of Geosciences, Princeton University, Princeton, USA (*09/02*).

29. **"Thermoelasticity of Minerals from First Principles"**, Department of Geological Sciences, University College London, London, UK (*09/02*).

28. **"Thermoelasticity of Minerals from First Principles"**, International Center for Theoretical Physics, Trieste, Italy (*05/02*).

27. **"First Principles Calculations in Mineral Physics"**, Department of Physics, Tokyo Institute of Technology, Tokyo, Japan (*03/02*).

26. **"First Principles Thermoelasticity of Minerals"**, Department of Earth and Planetary Sciences, Tokyo Institute of Technology, Tokyo, Japan (*03/02*).

25. **"Materials Theory and Mineral Physics"**, seminar speaker, Institute of Geophysics and Planetary Physics, UCLA, Los Angeles (*05/01*).

24. **"First Principles Thermoelasticity of Minerals: Applications to Mantle Minerals”**, Department of Earth Sciences, U. of Cambridge, Cambridge, UK (*11/00*).

23. **"First Principles Thermoelasticity of Minerals: Applications to Mantle Minerals"**, Colloquium speaker at the Department of Physics, University of Colorado, Boulder, CO (*04/00*).

22. **"First Principles Thermoelasticity of Minerals: Applications to Mantle Minerals"**, Colloquium speaker at the Department of Physics, SUNY-Stony Brook, NY (*11/99*).

21. **"New Phase and Gradual Coordination Change in Silica Under Pressure"**, Department of Physics (Condensed Matter Group), SUNY-Stony Brook, NY (*08/97*).

20. **"First Principles Studies of Minerals Under Pressure”**, Department of Physics (Condensed Matter Group), SUNY-Stony Brook, NY (*02/96*).

19. **"First Principles Studies of Minerals Under Pressure",** Department of Physics, Univ. of Coimbra, Portugal (*01/96*).

18. **"*Ab initio* Molecular Dynamics with Variable Cell Shape"**, Department of Materials Physics. Univ. of São Paulo, Brazil (*11/95*).

17. **"*Ab initio* Molecular Dynamics with Variable Cell Shape: Applications to $MgSiO_3$-perovskite and VO_2"**, Department of Physics, Univ. of Minnesota (*07/95*).

16. **"*Ab initio* Molecular Dynamics with Variable Cell Shape"**, Department of Geology and Geophysics, Univ. of Minnesota (*07/95*).

15. **"*Ab initio* Molecular Dynamics with Variable Cell Shape"**, Cray Research, Eagan, MN (*01/95*).

14. **"*Ab initio* Molecular Dynamics with Variable Cell Shape"**, Department of Physics (Cond. Matter Group), Univ. of Minnesota, (*11/94*).

13. **"*Ab initio* Molecular Dynamics with Variable Cell Shape: Applications to $MgSiO_3$-perovskite and VO_2"**, Max-Planck Institut, Stuttgart, Germany (*05/94*).

12. **"*Ab initio* Molecular Dynamics with Variable Cell Shape"**, Department of Physics, Keele, UK (*05/94*).

11. **"*Ab initio* Molecular Dynamics with Variable Cell Shape"**, Department of Physics, Aarhus, Denmark (*05/94*).

10. **"*Ab initio* Molecular Dynamics with Variable Cell Shape''**, Department of Physics, Bristol, UK (*05/94*).

9. **"*Ab initio* Molecular Dynamics with Variable Cell Shape*"***, Department o*f* Materials Sciences, Oxford, UK (*05/94*).

8. **"*Ab initio* Molecular Dynamics with Variable Cell Shape*"***, Department of Chemical Engineering and Materials Sciences, University of Minnesota, Minneapolis. USA (*05/94*).

7. **"*Ab initio* Molecular Dynamics with Variable Cell Shape"**, Department of Physics, Daresbury Laboratory, UK (*02/94*)

6. **"*Ab initio* Molecular Dynamics with Variable Cell Shape"**, Department of Solid State Physics, Univ. of Campinas, Campinas, Brazil (*8/93*).

5. **"*Ab initio* Molecular Dynamics with Variable Cell Shape: Application to $MgSiO_3$-perovskite''**, Laboratoire de Physique des Milieu Condenses Pierre et Marie Curie, Paris, France (*06/93*).

4. **"*Ab initio* Molecular Dynamics with Variable Cell Shape''**, The Royal Institution of Great Britain, Michael Faraday Laboratory, London , UK (*05/93*).

3. **"*Ab initio* Molecular Dynamics with Variable Cell Shape: Application to $M9SiO_3$-perovskite"**, Department of Physics, Brookhaven National Laboratory, Upton, NY (*03/93*).

2. **"*Ab initio* Molecular Dynamics with Variable Cell Shape: Applications to $MgSiO_3$-perovskite and VO_2"**, Fritz-Habber Institut, Berlin, Germany (*02/93*).

1. **"*Ab initio* Molecular Dynamics with Variable Cell Shape"**, Cavendish Laboratory, Cambridge. UK (*10/92*).

Invited talks given by group members

58. ***Dong-Bo Zhang*** - **"Phonon Quasiparticles and Thermal Conductivity in Crystalline Solids**", American Physical Society 2019 March Meeting, Boston, USA (*03/19*).

57. ***Koichiro Umemoto*** - **"Fate of $MgSiO_3$ Post-perovskite at TPa Pressures**", American Physical Society 2019 March Meeting, Boston, USA (*03/19*).

56. ***Gaurav Shukla***- **"Post-perovskite Transition in Iron Bearing Bridgmanite**", American Geophysical Union Fall 2016 Meeting, San Francisco, USA (*12/16*).

55. ***Koichiro Umemoto*** - **"Fate of $MgSiO_3$ Post-perovskite at TPa Pressures**", American Geophysical Union Fall 2016 Meeting, San Francisco, USA (*12/16*).

54. ***Koichiro Umemoto*** - **"Nature of the volume isotope effect in H_2O-ice**", 2015 IUCr High-Pressure Workshop, Campinas, SP, Brazil (*09/15*).

53. ***Michel Lacerta*** - **"Hybrid *ab initio*-experimental approach to modeling thermal properties of solids**", 2015 IUCr High-Pressure Workshop, Campinas, SP, Brazil (*09/15*).

52. ***Zhongqing Wu*** – "**Spin crossover in ferropericlase and lateral variations in Earth's lower mantle"**, American Geophysical Union Fall 2014 Meeting, San Francisco, USA (*12/14*).

51. ***Han Hsu*** – "**Intermediate-spin ferrous iron in the Earth's lower mantle?"**, American Geophysical Union Fall 2013 Meeting, San Francisco, USA (*12/13*).

50. ***Koichiro Umemoto*** – **"The volume isotope effect in H_2O ice under pressure"**, American Geophysical Union Fall 2013 Meeting, San Francisco, USA (*12/13*).

49. ***Tao Sun*** – **"Direct determination of electric current in Born-Oppenheimer molecular dynamics"**, American Geophysical Union Fall 2012 Meeting, San Francisco, USA (*12/12*).

48. ***Koichiro Umemoto*** – **"Fate of $MgSiO_3$ post-perovskite at ultra-high pressures"**, American Geophysical Union Fall 2012 Meeting, San Francisco, USA (*12/12*).

47. ***Koichiro Umemoto*** – **"Fate of $MgSiO_3$ post-perovskite at ultra-high pressures"**, International Symposium Nanoscience and Quantum Physics 2012, nanoPHYS'12, Tokyo, Japan *(12/12).*

46. ***Koichiro Umemoto*** – **"Fate of $MgSiO_3$ post-perovskite at ultra-high pressures"**, Gordon Research Conference, Invited Poster, University of New England, *USA (06/12).*

45. ***Koichiro Umemoto*** – **"Fate of $MgSiO_3$ post-perovskite at ultra-high pressures"**, Spring ACS Meeting Symposium "Quantum Chemistry for Geochemistry", San Diego, *USA (03/12).*

44. ***Koichiro Umemoto*** – **"New Multi-Mbar phases of H_2O and SiO_2"**, Exploring the Physics and Chemistry of Giant Planets on NIF Workshop, Livermore, *USA (12/11).*

43. ***Koichiro Umemoto*** – **"Two stage dissociation of $MgSiO_3$ post-perovskite"**, American Geophysical Union, Fall10 AGU Meeting, San Francisco, USA (*12/11*).

42. ***Han Hsu*** – "**Spin crossover and hyperfine interaction in LaCoO3"**, Department of Physics, North Dakota University State University, Fargo, USA (*05/11*).

41. ***Han Hsu*** – "**DFT+U calculations in iron-bearing minerals**", American Geophysical Union, Fall10 AGU Meeting, San Francisco, USA (*12/10*).

40. ***Koichiro Umemoto*** – **"Multi-Mbar phase transitions in minerals"**, International Mineralogical Association, Budapest, Hungary (*08/10*).

39. ***Koichiro Umemoto*** – **"First-principles investigation of order-disorder phase boundary in ice"**, Goldschmidt 2010 (keynote talk), Knoxville, USA, (*06/10*).

38. ***Han Hsu*** – "**Spin-state crossover in mantle minerals**", Electronic Structure 2010, Austin, USA (*06/10*).

37. ***Han Hsu*** – "**Spin states and hyperfine interactions of iron in (Mg,Fe)SiO_3 perovskite under pressure**", American Geophysical Union, Fall09 AGU Meeting, San Francisco, USA (*12/08*).

36. ***Koichiro Umemoto*** – **"Multi-Mbar phase transitions in minerals"**, American Geophysical Union, Fall09 AGU Meeting, San Francisco, USA (*12/09*).

35. ***Koichiro Umemoto*** – **"Multi Mbar phase transitions in minerals"**, MSA Short Course: Theoretical and Computational Methods in Mineral Physics: Geophysical Applications, Berkeley, USA (*12/09*).

34. ***Koichiro Umemoto*** – **"Order disorder phase boundary in ice VII-VIII investigated by first principles"**, Minnesota Supercomputing Institute, Scientific Computation Seminar Series, Minneapolis, USA (*11/09*).

33. ***Koichiro Umemoto*** – **"Spin transition in ferromagnesium silicate perovskite in the mantle"**, AGU Joint Assembly – Meeting of the Americas, Toronto, Canada (*05/09*).

32. ***Koichiro Umemoto*** – **"Post-postperovskite transitions"**, American Geophysical Union, Fall08 AGU Meeting, San Francisco, USA (*12/08*).

31. ***João Francisco Justo*** – **"Spin transition in ferromagnesium silicate perovskite in the mantle"**, Onsen Workshop on "Transport Properties in the Mantle", Yunishigawa, Japan (*10/08*).

30. ***Koichiro Umemoto*** – **"Spin transition in ferromagnesium silicate perovskite in the mantle"**, Onsen Workshop on "Transport Properties in the Mantle", Yunishigawa, Japan (*10/08*).

29. ***Cesar R. S. da Silva*** **– "VLab: a service oriented architecture for first principles computations of planetary materials properties"**, American Geophysical Union, Fall07 AGU Meeting, San Francisco, USA (*12/07*).

28. ***Cesar R. S. da Silva*** **– "VLab: a service oriented architecture for first principles computations of planetary materials properties"**, 2nd ***VLab*** Workshop, Minneapolis, USA (*08/07*).

27. ***Koichiro Umemoto*** – **"Spin Transition in ferrous iron in ferrosilicate perovskite"**, 2nd ***VLab*** Workshop, Minneapolis, USA (*08/07*).

26. ***Koichiro Umemoto*** – **"Ultrahigh pressure forms of ABX_3-type compounds"**, Woskshop of the Center of the Study of Matter at Extreme Conditions, CSMEC, Miami, USA (*04/07*).

25. ***Zhongqing Wu*** - **"P-V-T relations in MgO: an ultrahigh pressure scale for planetary sciences applications"**, American Geophysical Union, Fall06 AGU Meeting, San Francisco, USA (*12/06*).

24. ***Koichiro Umemoto*** – **"Order disorder transition in H_2O self-clathrates"**, American Geophysical Union, Fall06 AGU Meeting, San Francisco, USA (*12/06*).

23. ***Koichiro Umemoto*** – **"Minerals at condition of the giant's interiors"**, General Meeting of the International Mineralogical Association, Kobe, Japan *(07/06*).

22. ***Koichiro Umemoto*** – "**Dissociation of $MgSiO_3$ in the Gas Giants and in Terrestrial Exoplanets**", General Assembly, Spring AGU Meeting, Baltimore (*04/06*).

21. ***Koichiro Umemoto*** – "**Dissociation of $MgSiO_3$ in the Gas Giants and in Terrestrial Exoplanets**", Seminar, Department of Physics, U. of Nevada, University, Las Vegas, USA (*03/05*).

20. ***Stefano de Gironcoli*** (collaborator from Trieste), **"Spin Transition in Iron Doped Minerals Under Pressure"**, American Physical Society, Baltimore (*03/06*).

19. ***Taku Tsuchiya*** – **"Spin Transition in Magnesiowustite in Earth's Lower Mantle**", Japan Geosciences Union, Spring06 Meeting, Makuhari, Japan (*05/06*).

18. ***Koichiro Umemoto*** – "**Dissociation of $MgSiO_3$ in the Gas Giants and in Terrestrial Exoplanets**", American Geophysical Union, Spring06 AGU Meeting, Joint Assembly, Baltimore, USA (*05/06*).

17. ***Koichiro Umemoto*** – "**Phase Transformation in $MgSiO_3$ in the Gas Giants and in Terrestrial Exoplanets**", American Geophysical Union, Fall05 Meeting, San Francisco, USA (*12/05*).

16. ***Taku Tsuchiya*** – "**Post-perovskite Investigated by First Principles**", American Geophysical Union, Fall05 Meeting, San Francisco, USA (*12/05*).

15. ***Koichiro Umemoto*** – "**Dissociation of $MgSiO_3$ in the Gas Giants and in Terrestrial Exoplanets**", Condensed Matter Physics Seminar, Department of Physics, Stony Brook University, Stony Brook, USA (*11/05*).

14. ***Koichiro Umemoto*** – **"Dissociation of $MgSiO_3$-post-perovskite: Significance for the Solar Giants and Exoplanets",** International Workshop on the Post-Perovskite Phase Transition in the Earth's Deep Mantle, Tokyo, Japan *(10/05).*

13. ***Taku Tsuchiya*** – **"Spin Transition in Magnesiowustite in Earth's Lower Mantle"**, International Workshop on the Post-Perovskite Phase Transition in the Earth's Deep Mantle, Tokyo, Japan *(10/05).*

12. ***Koichiro Umemoto*** – **"Dissociation of MgSiO3-post-perovskite: Significance for the Solar Giants and Exoplanets",** 1st ***Vlab*** Workshop, 2005, Minneapolis, USA *(7/05).*

11. ***Taku Tsuchiya*** – **"Spin Transition in Magnesiowustite in Earth's Lower Mantle"**, 1st ***Vlab*** Workshop, 2005, Minneapolis, USA *(7/05).*

10. ***Taku Tsuchiya*** – **"$MgSiO_3$ Post-Perovskite at D" conditions"**, Goldschmidt Conference 2005, Moscow, USA *(5/05).*

9. ***Taku Tsuchiya*** – **"$MgSiO_3$ Post-Perovskite at D" conditions"**, American Geophysical Union, 2004 Fall Meeting, San Fransisco, USA *(12/04).*

8. ***Taku Tsuchiya*** – **"Post-Perovskite Transition in $MgSiO_3$"**, American Geophysical Union, Montreal, Canada *(05/04).*

7. ***Koichiro Umemoto*** - **"Low ↔ High Density Transformations in H_2O-ice"**, American Geophysical Union, San Francisco, USA (*12/03).*

6. ***Koichiro Umemoto*** – **"Low ↔ High Density Transformations in H_2O-ice"**, IUCr/COMPRES Workshop, Berkeley, USA (*12/03).*

5. ***Koichiro Umemoto*** - **"Amorphization and Other Pressure Induced Anomalies in H_2O-ice"**, 15th Annual Workshop on Recent Developments in Electronic Structure Methods (Electronic Structure'03), Minneapolis, USA (*5/03).*

4. ***Bijaya B. Karki*** - **"Thermoelastic Properties of Mantle Minerals and Geophysical Implications"**, Mardi Gras Conference on Multiscale Simulation, Theoretical and Experimental Approaches to Deformation, Fatigue, and Fracture, Baton Rouge, USA (*2/01*).

3. ***Bijaya B. Karki*** - **"First Principles Thermoelasticity of Minerals"**, XIX European Crystallographic Meeting. Symposium on Theoretical Studies of Minerals and Minerals' Properties, Nancy, France (*8/00*).

2. ***Bijaya B. Karki*** - **"First Principles Thermoelasticity of Minerals: Geophysical Implications"**, XXXI International Geological Congress, Symposium on Physics and Chemistry of Minerals, Rio de Janeiro, Brazil (*8/00*).

1. ***Bijaya B. Karki*** - **"First Principles Thermoelasticity of Minerals: Geophysical Implications"**, Twelfth Annual Workshop on Recent Developments in Electronic Structure Methods (Electronic Structure 2000), Atlanta, USA (*5/00*).