RENATA M. M. WENTZCOVITCH
Professor of Applied Physics and Materials Science
Department of Applied Physics and Applied Mathematics
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A. FIELD OF SPECIALIZATION

Materials Science and Engineering/Earth and Environmental Sciences with a focus on:
• Computational Materials Physics
• Simulation of Matter in 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)	the 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 and Visiting Positions

• Visiting Professor, Instituto de Astronomia, Geofísica, e Ciências Atmosféricas, Universidade de São Paulo, Brazil (*05/2024-08/2024*).

• Harry Hess Visiting Professor, Department of Geosciences, Princeton University, Princeton, (*02/2024-04/2024*).

• Visiting Researcher, Earth-Life Science Institute, Tokyo Institute of Technology, and University of Tokyo, Japan (*01/2024*).

• Visiting Scholar, Center for Computational Quantum Physics, Flatiron Institute, New York (*09/2023-12/2023*).

• Visiting Scientist, Department of Geosciences, Utrecht University, Utrecht, The Netherlands (*07/2023*).

• Principal Investigator at the Earth-Life Science Institute (ELSI), World Premier International Research Institute (WPIRI) of the JSPS, Tokyo Institute of Technology, Tokyo, Japan *(10/2012-2022).*

• Adjunct Research Scientist, Lamont Doherty Earth Observatory, Columbia University (*08/2016-*• 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 2022, 2023, 2025* – Lecturer in *Materials Thermodynamics and Phase Diagrams* (MSAE E4201 and E3201, CVN class). Junior-level course on Thermodynamics (class size, ~45 students).
- *Spring 2018, 2019, 2020, 2021* – 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).
- *Fall 2020, 2021* – Organizer of Seminar in Geophysics Series *"Cool Topics in Geophysics"* (MSAE E3011). Graduate-level seminar series in the Department of Earth and Environmental Sciences (~16 participants).
- *Fall 2022, 2024* – Organizer of Seminar Series *"Materials Simulations in Earth and Planetary Sciences"* in the Department of Applied Physics and Applied Mathematics. Weekly virtual graduate-level seminar series open to the broad mineral physics and Earth Sciences community with invited speakers from Columbia and other institutions (~16-20 participants).

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).

3. 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).

E. PERSONNEL SUPERVISION

1. Current Advisees

Hongjin Wang (01/2021-) Graduate student (PhD track) in the Department of Applied Physics and Applied Mathematics, Materials Science Program.

Tianqi Wan (04/2025-) Postdoctoral Fellow, Lamont-Doherty Earth Observatory, Columbia University.

Jessica Santos Rego (01/2025-) Post-doc with São Paulo State Research Foundation (FAPESP) Fellowship, Department of Applied Physics and Applied Mathematics, Columbia University.

2. Alumni: Post-doctoral fellows

Wenhui Duan (*1996-99*) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota. Currently, Professor and Chair, Physics Department, Tsinghua University, Beijing. APS Fellow. Member of the Chinese Academy of Sciences (*2016*), China.

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

Bijaya Karki (*1997-2001*) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota. 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*) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota. Currently, staff scientist at Nippon Electric Glass (NEG), Kyoto, Japan.

João Francisco Justo (research associate, *2007-08*) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota. Currently, Professor, Electrical Engineering, Escola Politécnica, U. of São Paulo, SP, Brazil.

Taku Tsuchiya (JSPS Fellow, *2003-2005*) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota. Currently, Professor of Mineral Physics and Director, Center for Geodynamical Research, Ehime University, Japan.

Jun Tsuchiya (JSPS Fellow, *2003-05*) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota. Currently, Professor of Mineral Physics, Osaka University, Japan.

Razvan Caracas (*2003-04*) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota. Currently, Professor of Mineral Physics, Université Paris Cite, Institut de Physique du Globe de Paris, CNRS, Paris, France.

Amel Laref (*2006-07*) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota; Research Associate, King Saud University, Department of Physics and Astronomy, Riyadh, Saudi Arabia. Moved to the private sector in 2010.

Pierre Carrier (*2006-08*) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota. Currently, applications and benchmarking analyst at Cray Inc., Minneapolis, MN, USA.

Zhongqing Wu (*2005-08*) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota. Currently, Professor in the Department of Earth and Space Sciences, U. of Science and Technology of China, Hefei, China.

Dipta Bahnu Ghosh (*2008-09*) Software Engineer, Microsoft, Seattle, US.

Yonggang Yu (*2010-11*) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota. *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, a staff member at NOAA, Earth System Research Lab, Global Systems Division, Boulder, CO, USA.

Maribel Núnez-Valdéz (*2011-13*) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota. Currently, W2-Professor, Helmholtz-Zentrum, Deutsches GeoForschungsZentrum (GFZ), Potsdam, Germany.

Tao Sun (*2011-13*) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota. Currently, 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. Winner of *1,000 Youth Talents of China* competition.

Dong-Bo Zhang (*2011-14*) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota. Currently, Professor, Department of Physics, Beijing Normal University, Beijing, China (*04/14*). Winner of *1,000 Youth Talents of China* competition.

Fawei Zheng (*2014-15)* Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota. Currently, Associate Professor, Computational Condensed Matter Physics, Institute for Applied Mathematics and Computational Physics, Chinese Academy of Engineering Physics, Beijing, China.

Mehmet Topsakal (2013-16) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota. Currently, Research Staff, Nuclear Science and Technology Department, Brookhaven National Laboratory, Upton, NY, USA.

Gaurav Shukla (*2016*) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota. Currently, Associate Professor, Department of Earth Sciences, Indian Institute of Science Education and Research, IISER-Kolkata, Mohanpur, India.

Pedro da Silveira (*2014-16)* Lead senior software engineer, Apple Inc., Austin, TX, USA

Joelson Cott-Garcia (2016) Post-doc, Department of Chemical Engineering and Materials Science, University of Minnesota, Business/Materials Development Researcher, Nissan Chemical America Corporation, Santa Clara, CA, USA.

Kanchan Sarkar (09/2014-17) Research Associate in Chemical Engineering and Materials Science, University of Minnesota; *(09/2017-19)* Research Associate, Department of Applied Physics and Applied Mathematics, Columbia University; currently research scientist at the Institute of Theoretical Chemistry, University of Ulm.

Michel Marcondes-Lacerda (05/2017-19) Post-doc, Lamont-Doherty Earth Observatory, Columbia University; currently Investment Software Engineer, Banco do Brasil, SP, Brazil.

Yang Sun (11/2019-2021) Research Associate, Department of Applied Physics and Applied Mathematics, Columbia University; currently Associate Professor, Department of Physics, Xiamen University, Xiamen, China.

Wenjie Lei (04/2021-10/22) Post-doc, Department of Earth and Environmental Sciences, Columbia University; currently AI specialist at Google, Silicon Valley.

3. 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, Lead senior software engineer at Apple Inc., Austin, TX.

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

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

Tian Qin (PhD, Earth Sciences, *2014-19*), Senior software engineer, Shenzhen Bay Lab, Shenzhen, China.

Ziyu Cai (MSc, Applied Physics and Applied Mathematics, Materials Science Program, *2018-19).* Currently, data scientist at Infineum, Shanghai, China.

Tianqi Wan (MSc, Applied Physics and Applied Mathematics, Materials Science Program, *2018-19).* Currently, GRA at the Department of Applied Physics and Applied Mathematica, Columbia University.

Hongjin Wang (MSc, Applied Physics and Applied Mathematics, Materials Science Program, *2018-19);* MSc (*2020-21*), Department of Computer Science, Columbia University.

Chenhui Yang (MSc, Applied Physics and Applied Mathematics, Materials Science Program, *2018-19).* Currently, GRA is in the Department of Applied Physics and Applied Mathematics, University of Virginia.

Jiayang Wang (MSc Applied Physics and Applied Mathematics, Materials Science Program, *2020-21).* Currently, GRA in Department of Materials Science, Penn State University.

Yuanchen Gao (MSc, Applied Physics and Applied Mathematics, Materials Science Program, *2020-21).* Currently, GRA in the Department of Applied Physics and Applied Mathematics, University of Virginia.

Chaoxuan Gu (MSc, Applied Physics and Applied Mathematics, Materials Science Program, *2021-22).* Currently, GRA in the Department of Materials Science, Brown University.

Zhen Zhang (PhD, Applied Physics and Applied Mathematics, Applied Physics Program, *2018-23*). Currently, Post-doc in the Department of Physics, Iowa State University, Ames, IA.

Qi Zhang Graduate (MSc track from *2017-18,* PhD, Applied Physics and Applied Mathematics, Materials Science Program, *2019-24*). Currently postdoc in the Applied Physics and Applied Mathematics Department, Columbia University. Currently, postdoc at Los Alamos National Laboratory.

Chenxing Luo (MSc (*2018-19*) and PhD (*2019-24*), Applied Physics and Applied Mathematics, Materials Science Program, Columbia University. Currently, *Harry Hess Post-doctoral Fellow*, Department of Geosciences, Princeton University.

Sangjoon Lee (MSc track from *2023-24*) Graduate student in the Department of Applied Physics and Applied Mathematics, Materials Science Program.

Jingyi Zhuang (MSc (*2018-19*) Applied Physics and Applied Mathematics, Materials Science Program, and PhD (*2019-24*), Department of Earth and Environmental Sciences, Columbia University. Currently, Software Engineer, Amazon AWS, Seattle, US.

Tianqi Wan (01/2020-) Graduate student (PhD track) in the Department of Applied Physics and Applied Mathematics, Materials Science Program. Currently, Postdoctoral Fellow at Lamont-Doherty Earth Observatory, Columbia University.

4. 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 at 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.

5. Alumni: Visiting students and researchers

Jessica Santos Rego – Visiting Scientist from student from Physics Institute, University of São Paulo (USP), – São Paulo, Brazil *(2025)*. Currently a postdoc at USP.

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.

F. PUBLICATIONS

(See separate file)

G. HONORS AND AWARDS

• Harry Hess Visiting Professorship at Princeton University (*02/2024 to 04/2024*)
• President-Elect (*2023-24*), President (*2025-26*), Past-President (*2027-2028*), Mineral and Rock Physics Section, American Geophysical Union.
• Vice-Chair, Chair-Elect, Chair, Past-Chair, Division of Computational Physics, American Physical Society (*2017-20*)
• Outstanding Referee for Physical Review B (*2021*)
• Wilhelm Heraeus Visiting Professorship Award, University of Frankfurt (€40,000) (*2015-16*)
• Member, 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.

H. INVITED PRESENTATIONS

(See separate file)

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

1) Co-organizer with Carlos Alberto Moreno Chaves, Caetano Miranda, John Hernlund, Alexandre Reily Rocha, and Victor Sacek, Mineral and Rock Physics Sessions, *Materials Simulations in Earth and Planetary Sciences*, South America Institute for Fundamental Research, IFT, UNESP, São Paulo, BR *(06/2025).*

2) Co-organizer with Bijaya Karki, Dipta Ghosh, and Han Hsu, Mineral and Rock Physics Sessions, *Exploring Planetary Materials through Computational Simulations and Data Analytics*, American Geophysical Union Fall Meeting, Washington DC, USA *(12/2024).*

3) Co-organizer with Bijaya Karki, Dipta Ghosh, and Han Hsu, Mineral and Rock Physics Sessions, *Exploring Planetary Materials through Computational Simulations and Data Analytics*, American Geophysical Union Fall Meeting, Chicago, USA *(12/2022).*

4) Organizer, Town Hall Meeting, *A Science Gateway for Mineral and Rock Physics*, American Geophysical Union Fall Meeting, San Francisco, USA *(12/2023).*

5) Co-organizer with Bijaya Karki, Dipta Ghosh, and Han Hsu, Mineral and Rock Physics Sessions, *Exploring Planetary Materials through Computational Simulations and Data Analytics*, American Geophysical Union Fall Meeting, San Francisco, USA *(12/2023).*

6) Organizer, Workshop *Computational Quantum Thermodynamics*, Columbia Global Center in Nairobi, Kenya *(11/2022).* http://mineralscloud.com/events/2022/workshop-thermodynamics

7) Chair, *International Conference in Computational Physics*, co-Chairs James R. Chelikowsky, Ellen Zweibel, Feliciano, Giustino, CCP'22, a virtual conference hosted by UT-Austin, TX, USA, (*08/2022*). https://ccp2022.oden.utexas.edu/

8) Chair, *International Workshop on Recent Developments in Electronic Structure Methods*, *ES22*, co-Organizers David Reichman, Raquel Queiroz, Timothy Berkelbach, Johannes Flick, hosted by Columbia University and Flatiron Institute, New York, NY, USA, (*06/2022*). https://www.apam.columbia.edu/international-workshop-recent-developments-electronic-structure-es22-1

9) Co-organizer, *US-Africa Initiative in Electronic Structure Conference*, co-organizers Richard Martin, Omololu Akin-Ojo, virtual, New York, USA (*06/2022*). https://usafricainitiative.org/MayWorkshop2022/

10) Co-organizer with Bijaya Karki, Dipta Ghosh, and Koichiro Umemoto, Mineral and Rock Physics Sessions, *Advances in Computational Mineral Physics*, American Geophysical Union Fall Meeting, New Orleans, USA *(12/2021).*

11) Co-organizer, *US-Africa Initiative in Electronic Structure Conference*, co-organizers Richard Martin, Omololu Akin-Ojo, ICTP-EAIFR, Kigali, Rwanda (*06/2021*).

12) Co-organizer, (virtual) Mini-Workshop of *US-Africa Initiative in Electronic Structure Conference*, APS March Meeting'21, co-organizers Richard Martin, Omololu Akin-Ojo, ICTP-EAIFR, Kigali, Rwanda (*06/2021*). https://march.aps.org/events/workshop-for-the-us-africa-initiative-in-electronic-structure/

13) Co-organizer with Han Hsu, Sally Tracy, and Elizabeth Thompson, Mineral and Rock Physics Sessions, *Connecting Mineral Properties to Planetary Models*, American Geophysical Union Fall Meeting, Virtual Meeting, USA *(12/2020).*

14) Lead-organizer, with co-organizers Kei Hirose, Paul Tackley, and Jeroen Tromp, Union Sessions, *Emergent views on Earth Deep Interior*, American Geophysical Union Fall Meeting, San Francisco, USA *(12/2019).*

15) Lead-organizer, *Room Temperature Superconductivity in Superhydrides at Extreme Pressures*, co-organizer Russell Hemley, Division of Computational Physics Invited Symposium, APS March Meeting 2020, Boulder, USA (*03/2020*). (Cancelled)

16) Program Committee Member, Division of Computational Physics, APS March Meeting 2020, Boulder (*03/2020*).

17) Lead-organizer, with co-organizers Kei Hirose, Paul Tackley, and Jeroen Tromp, Union Sessions, *Emergent view on Earth Deep Interior*, American Geophysical Union Fall Meeting, San Francisco, USA *(12/2019).*

18) Co-organizer, with Koichiro Umemoto, and Han Hsu, Mineral and Rock Physics Sessions, *Advances in Computational Mineral Physics and Geochemistry*, American Geophysical Union Fall Meeting, San Francisco, USA *(12/2019).*

19) Program Committee and International Advisory Committee member for the *27th AIRAPT International Conference on High-Pressure Science and Technology*, Rio de Janeiro. (*08/2019*).

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

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

22) 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*).

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

24) 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*).

25) 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).*

26) 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*).

27) 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*).

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

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

30) 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)*.

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

32) 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)*.

33) 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).*

34) 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).*

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

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

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

38) 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).*

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

40) 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).*

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

42) 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.

43) 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).*

44) 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).*

45) 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).*

46) 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*).

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

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

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

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

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

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

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

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

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

56) 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).*

57) 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*).

58) 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 on the Board of Directors of the Great Lakes Consortium for Petascale Computing – The Blue Waters Project (*2017-2019*)
- Data Science Institute – a member of the "Frontiers in Computing Systems" working group.
- Member of the "Habitable Planet" working group at the Earth Institute (*2021-2023*).

• *Department of Physics and Astronomy*

- Faculty Recruiting Committee in Theoretical Condensed Matter Physics (*Spring-2021*)

• *School of Engineering and Applied Sciences*

- Co-Chair of the Faculty Recruiting and Pipeline Breakout Group of the Diversity, Equity, and Inclusion Commission (*Fall-2020 to Spring-2021*)
- APAM Representative in the SEAS-DEI Committee (*Fall-2021 to Spring-2024*)

• *APAM Department*

- Undergraduate advisor for the Materials Science Program (*2022-2024*)
- MSE Oral Exam Committee Chair (*Spring-2023, Spring-2024, Spring-2025*)
- 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 (*2019-present*)
- APAM representative in SEAS Diversity, Equity, and Inclusion Committee (*Fall 2021-2024*).

• *Department of Earth and Environmental Sciences*

- Faculty Recruiting Committee (*Spring-2018*)
- Target of Opportunity Faculty Recruiting Committee (*Spring-2019-2022*)
- Member of the Diversity Equity and Inclusion Committee (*Spring-2022-Fall-2023*)

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*)
- 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):*
  - Member of APS Honors Task Force (06/*2022-08/2023*)
  - Member of the International Committee of the APS/DCOMP (*01/2024-10/2024*)
  - Committee on International Freedom of Scientists (*01/2022-present*)
  -APS/GSCCM – Neil Ashcroft Early Career Award Endowment Committee *(2021-2022)*
  -Vice-Chair (*2017*), Chair-Elect (*2018*), Chair (*2019*), Past-Chair (*2020*), Division of Computational Physics (APS/DCOMP)
  -Chair of the Fellowship Committee (APS/DCOMP) (*2020*)
  - Nominating Committee (APS/DCOMP) (*2021*)
  -Aneesur Rahman Prize Endowment Fundraising Committee *(2018-2022*)
  -APS March Meeting, DCOMP Program Committee member *(2003,2018-2021,* Chair in *2019)*
  -DCOMP - Aneesur Rahman Prize Selection Committee, Vice-Chair *(2012*), Chair (*2016*)
  -DCOMP – Member-at-large of the Executive Committee (*2001-03*)
  -Committee on the Status of Women in Physics, site visit team member, U. of Washington *(2005)*
• *Service to the American Geophysical Union (AGU):*
  - Science Advisor for *Eos: Earth and Space Sciences News* (*01-2025 to 12-2027*)
  - President-Elect (*2023-24*), President (*2025-26*), Past-President (*2027-2028*), Mineral and Rock Physics Section, American Geophysical Union.
  - Mineral and Rock Physics (MRP) Fellowship Committee member *(2021-2022 (regular), 2023-2024 (Chair)*)
  - Study of Earth's Deep Interior (SEDI) Fellowship Committee member *(2021-2022 (regular), 2023 (Chair)*)
• *Service to the Mineralogical Society of America*

-Distinguished Public Service Medal Selection Committee (*2020*)

• *Service to the International Association for High-Pressure Research, AIRAPT*

-Executive Committee Member (*07/2023-present*)

-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*)

-University of Minnesota Elector and Representative (*2003-2016*)

• *Review Panels:*

-National Science Foundation (CISE)**:** Review panel member for CSSI/Elements *(2024)*

-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*

- Science Advisor for Eos-Earth and Space Sciences News (*01-2025-present*)

- Editor, Journal of Geophysical Research: Machine Learning & Computation (*2024-present*)

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

- 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

~250+ publications in peer-reviewed journals, 18 conference proceedings; 3 books edited; one instruction video; Google Scholar: 50,380+ citations; h-index 73; i10-index 211 (*04/07/2025*) (including surname misspellings as Wentzovitch and Wentzowitch).

In preparation (underlined names are current or former group members)

S1. T. Wan, Y. Sun, R. M. Wentzcovitch, **Spin state and antiferromagnetic ordering of iron in δ-Fe_3O_4**, in preparation (2024).

S2. N. Huang, Y. Fang, F. Zheng, Y. Sun, C.-Z. Wang, K.-M. Ho, R. M. Wentzcovitch, **Exploring novel stable Fe-Si-O phases at TeraPascal Pressures,** in preparation (2024).

S3. S.-C. Huang, K. Sarkar, R. M. Wentzcovitch, H. Hsu, **Orbital-ordered ferromagnetic insulating state in tensile-strained $SrCoO_3$ thin films**, under revision for *Phys. Rev. Lett.* (2024). https://arxiv.org/abs/2211.10404

Under review

S4. T. Wan, Y. Sun, and R. M. Wentzcovitch, **Spin state of iron in $I\bar{4}2d$-type Mg_2SiO_4 at ultra-high pressure**, under review, *Phys. Rev. B* (2025).

S5. Z. Wu, C. Gao, F. Zhang, S. Wu, K.-M. Ho, R. M. Wentzcovitch, and Y. Sun, ***Ab initio* superionic-liquid phase diagram of $Fe_{1-x}O_x$ under inner core conditions**, *Phys. Rev. Lett.*, under review (2025). https://arxiv.org/pdf/2410.23557

S6. T. Wan, C. Luo, Z. Zheng, Y. Sun, and R. M. Wentzcovitch, **Ferroelasticity, shear modulus softening, and the tetragonal↔cubic transition in davemaoite**, *Communications Earth & Environment,* under review (2025).

S7. L. Wei, K.-M. Ho, R. M. Wentzcovitch, Y. Sun, **The Fe-Ni phase diagram and the Earth's inner core structure**, *Science Advances*, under review (2025).

2025

249. C. Gao, R. M. Wentzcovitch, K.-M. Ho, and Y. Sun**, Understanding the two-step nucleation of iron at Earth's inner core conditions: a comparative molecular**

dynamics study, *Phys. Rev. B* **111**, 134104. DOI: 10.1103/PhysRevB.111.134104 (2025).

248. E. Camporeale, R. Marino, T. Berger, Y. Chen, D. Folini, G. Fox, X. Li, D. Lucas, S. Tobias, M. Reichstein, J. Rundle, C. Shen, R. Wentzcovitch, and Y. Wen, **Thank you to our peer reviewers in 2024**, *J. Geophys. Res.- Machine Learning and Computation* **2**, e2025JH000681. DOI: e2025JH000681 (2025).

2024

247. H. Wang, C. Luo, and R. M. Wentzcovitch, **Machine learning potentials for serpentines**, *J. Geophys. Res. Machine Learning and Computations* **1**, e2024JH000434. DOI: 10.1029/2024JH000434 (2024). https://arxiv.org/pdf/2409.16402

246. C. Luo, Y. Sun, and R. M. Wentzcovitch, **Elasticity and acoustic velocities of δ-AlOOH at extreme conditions: a methodology assessment**, *Phys. Rev. Materials* **8**, 103601 (2024). DOI: 10.1103/PhysRevMaterials.8.1 https://arxiv.org/pdf/2406.13804

245. Z. Zhuang and R. Wentzcovitch, **Fe^{2+} partitioning in Al-free pyrolite: consequences for seismic velocities and heterogeneities**, *Geophys. Res. Lett.* **51**, e2024GL108967 (2024). DOI: 10.1029/2024GL108967 https://arxiv.org/pdf/2405.11830

244. F. Wu, S. Wu, C.-Z. Wang, K.-M. Ho, R. M. Wentzcovitch, Y. Sun, **Melting Temperature of Iron Under the Earth's Inner Core Condition from Deep Machine Learning**, *Geoscience Frontiers* **51**, 101925 (2024). DOI: 10.1016/j.gsf.2024.101925 https://arxiv.org/abs/2404.17852

243. F. Wu, Y. Sun, T. Wan, S. Wu, and R. M. Wentzcovitch, **Deep-learning-based prediction of the tetragonal to cubic transition in davemaoite**, *Geophys. Res. Lett*. **51**, e2023GL108012 (2024). DOI: 10.1029/2023GL108012 https://arxiv.org/html/2401.14588v1

242. H. Wang, C. Luo, and R. M. Wentzcovitch, **Ab initio study on the stability and elasticity of brucite**, *Phys. Rev. B* **109**, 214103 (2024). DOI: 10.1103/PhysRevB.109.214103 https://arxiv.org/abs/2311.17268

241. T. Wan, C. Luo, Y. Sun, and R. M. Wentzcovitch, **Thermoelastic properties of bridgmanite using Deep Potential Molecular Dynamics**, *Phys. Rev. B* **109**, 094101 (2024). DOI: 10.1103/PhysRevB.109.094101 https://arxiv.org/abs/2307.07127

240. C. Luo, Y. Sun, and R. M. Wentzcovitch, **Probing the state of hydrogen in δ-AlOOH at mantle conditions with machine learning potential**, *Phys. Rev. Research* **6**, 013292 (2024). DOI: 10.1103/PhysRevResearch.6.013292 https://arxiv.org/abs/2309.06712

239. L. Cobden, J. Zhuang, W. Lei, R. M. Wentzcovitch, J. Trampert, and J. Tromp, **Full-waveform tomography reveals iron spin crossover in Earth's lower mantle**, *Nature Communications* **15**, 1961 (2024). DOI: 10.1038/s41467-024-46040-1 https://arxiv.org/abs/2303.05476

238. Y. Sun, M. I. Mendelev, F. Zhang, Z. Liu, X. Liu, B. Da, C.-Z Wang, R. M. Wentzcovitch, and K.-M. Ho, **Unveiling the effect of Ni on the formation and structure of Earth's inner core**, *Proceedings of the National Academy of Sciences of the*

USA **121**, e2316477121 (2024). DOI: 10.1073/pnas.231647712 https://arxiv.org/abs/2308.04280

2023

237. Y. Fang, Y. Sun, R. Wang, F. Zheng, F. Zhang, S. Wu, C.-Z. Wang, R. M. Wentzcovitch, K.-M. Ho, **Structural prediction of Fe-Mg-O compounds at Super-Earth's pressures**, *Phys. Rev. Research* **7**, 113602 (2023). DOI: 10.1103/PhysRevMaterials.7.113602 https://arxiv.org/abs/2307.03632

236. L. Tang, C. Zhang, Y. Sun, K.-M. Ho, R. M. Wentzcovitch, and C.-Z. Wang, **Structure and dynamics of $Fe_{90}Si_3O_7$ liquids close to Earth's liquid core conditions**, *Physical Review B* **108**, 064104 (2023). DOI: 10.1103/PhysRevB.108.064104 http://arxiv.org/abs/2303.03585

235. D. Zeng, D. Zhang, D. Lu, P. Mo, Z. Li, Y. Chen, M. Rynik, L. Huang, Z. Li, S. Shi, Y. Wang, H. Ye, P. Tuo, J. Yang, Y. Ding, Y. Li, D. Tisi, Q. Zeng, H. Bao, Y. Xia, J Huang, K. Muraka, Y. Wang, J. Chang, F. Yuan, S. L. Bore, C. Cai, Y. Lin, B. Wang, J. Xu, J.-X. Zhu, C. Luo, Y. Zhang, R. E. A. Goodall, W. Liang, A. K. Singh, S. Yao, J. Zhang, R. Wentzcovitch, J. Han, J. Liu, W. Jia, D. M. York, W. E, R. Car, L. Zhang, and H. Wang, **DeePMD-kit v2: A software package for Deep Potential models**, *J. Chem. Phys.* **159**, 054801 (2023). DOI: 10.1063/5.0155600 https://arxiv.org/pdf/2304.09409

234. Z. Zhang, Y. Sun, and R. M. Wentzcovitch, **PBE-GGA predicts the B8↔B2 phase boundary of FeO under Earth's core pressures**, *Proc. Nat. Acad. Sc. USA* **120**, e2304726120 (2023). DOI: 10.1073/pnas.2304726120 https://arxiv.org/abs/2211.15052

233. H. Wang, J. Zhuang, Z. Zhang, Q. Zhang, and R. M. Wentzcovitch, **`pqm`: a Python package for free-energy calculations within the phonon gas model**, *Comp. Phys. Comm.* **28**, 108845 (2023). DOI: 10.1016/j.cpc.2023.108845 https://arxiv.org/abs/2303.11583

232. R. M. Wentzcovitch, J. Valencia Cardona, J. Zhuang, G. Shukla, and K. Sarkar, **The Post-perovskite transition in Al- and Fe-bearing bridgmanite: effects on seismic observables**, *J. Geophys. Res.* **128**, e2022JB025475 (2023). DOI: 10.1029/2022JB025475 https://arxiv.org/abs/2208.12207

231. Y. Sun, M. I. Mendelev, F. Zhang, Z. Liu, B. Da, C.-Z Wang, R. M. Wentzcovitch, and K.-M. Ho, ***Ab initio* melting temperatures of bcc and hcp iron under the Earth's inner core condition**, *Geophys. Res. Lett.* (2023). DOI: 10.1029/2022GL102447 https://arxiv.org/abs/2205.02290

230. Q. Zhang, C. Gu, J. Zhuang, and R. M. Wentzcovitch, **`express`: extensible, high-level workflows for swifter *ab initio* materials modeling**, *Comp. Phys. Comm.*, 108515 (2023). DOI: 10.1016/j.cpc.2022.108515 https://arxiv.org/abs/2109.11724

229 J. Liu, Y. Sun, C. Lv, F. Zhang, S. Fu, V. B. Prakapenka, C.-Z. Wang, K.-M. Ho, J.-F. Lin, R. M. Wentzcovitch, **Iron-rich Fe-O compounds at Earth's core pressures**, *The Innovation* **4**, 100354, (2023). DOI: 10.1016/J.XINN.2022.100354 https://arxiv.org/abs/2110.00524

2022

228. C. Luo, R. M. Wentzcovitch, and J. Tromp, **3rd order elastic coefficients and stress-dependent elasticity**, *Phys. Rev. B* **106**, 214104 (2022). DOI: 10.1103/PhysRevB.106.214104 https://arxiv.org/abs/2204.07608

227. Z. Zhang and R. M. Wentzcovitch, **Anharmonic thermodynamic properties and phase boundary across the post-perovskite transition in $MgSiO_3$,** *Phys. Rev. B* **106**, 054103 (2022). DOI: 10.1103/PhysRevB.106.054103 https://arxiv.org/abs/2204.13159

226. X. Deng, C. Luo, G. Abers, R. M. Wentzcovitch, and Z. Wu, **Elastic anisotropy of lizardite at subduction zone conditions**, *Geophys. Res. Lett.* **49**, e2022GL099712 (2022). DOI: 10.1029/2022GL099712 https://arxiv.org/abs/2209.09783

225. F. Zheng, Y. Sun, R. Wang, Y. Fang, F. Zhang, S. Wu, C.-Z. Wang, R. M. Wentzcovitch, K.-M. Ho, **Structure and motifs of iron oxides from 1 to 3 TPa**, *Phys. Rev. Materials* **6**, 043602 (2022). DOI: 10.1103/PhysRevMaterials.6.043602 https://arxiv.org/abs/2111.01305

224. C. Zhang, L. Tang, Y. Sun, K.-M. Ho, R. M. Wentzcovitch, and C.-Z. Wang, **Deep machine learning potential for atomistic simulations of Mg-Si-O systems under Earth's outer core conditions**, *Phys. Rev. Materials* 6, 063802 (2022). DOI: 10.1103/PhysRevMaterials.6.063802 https://arxiv.org/abs/2201.11835

223. T. Wan, Y. Sun, and R. M. Wentzcovitch, **Intermediate spin state and the B1-B2 transition in ferropericlase at Tera-Pascal pressures**, *Phys. Rev. Research*, **4**, 023078 (2022). DOI: 10.1103/PhysRevResearch.4.023078 https://arxiv.org/abs/2109.11008

222. C. Luo, K. Umemoto, and R. M. Wentzcovitch, ***Ab initio* investigation of H-bond disordering in δ-AlOOH**, *Phys. Rev. Research* **4**, 023223 (2022). DOI: 10.1103/PhysRevResearch.4.023223 https://arxiv.org/abs/2112.11369

221. Z. Zhang, D.-B. Zhang, S. Tao, R. M. Wentzcovitch, **The phonon quasiparticle method**, *Journal of Physics: Conference Series* **2207**, 012042 (2022). DOI: 10.1088/1742-6596/2207/1/012042 https://arxiv.org/abs/2112.11571

220. Y. Sun, J. Zhuang, and R. M. Wentzcovitch, **Thermodynamics of spin crossover in ferropericlase: an improved LDA+Usc calculation,** *Electronic Structure* **4**, 014008 (2022). DOI: 10.1088/2516-1075/ac522b https://arxiv.org/abs/2110.12637.

219. Y. Sun, F. Zhang, M. Y. Mendelev, R. M. Wentzcovitch, K.-M. Ho, **Two-step nucleation of the Earth's inner core**, *Proceedings of the National Academy of Sciences of the USA*, **119**, e2113059199, (2022). DOI: 10.1073/pnas.2113059119 https://arxiv.org/abs/2105.07296

2021

218. Z. Zhang, D.-B. Zhang, K. Onga, K. Ohta, K. Hirose, R. M. Wentzcovitch, **Thermal conductivity of cubic $CaSiO_3$–perovskite at lower mantle conditions**, *Phys. Rev. B* **104**, 184101, (2021). DOI: 10.1103/PhysRevB.104.184101 https://arxiv.org/abs/2005.08289s

217. Y. Fang, Y. Sun, R. Wang, F. Zheng, S. Wu, C.-Z. Wang, R. M. Wentzcovitch, K.-M. Ho, **Unconventional iron-magnesium compounds at tera-Pascal pressures,** *Phys. Rev. B* **104**, 144109 (2021). DOI: 10.1103/PhysRevB.104.144109 (2021). https://arxiv.org/abs/2104.07700

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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).
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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).

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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).

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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 >340 invited talks and seminars. They consistently present 20+ contributed talks/posters annually in APS, AGU, and other meetings.

Conferences and Workshops

141 "**Modeling Earth from Atomic to Global Scale,"** Symposium in Honor of Marvin L. Cohen, UC-Berkeley, USA (*03/25*).

140 "**Modeling Earth from Atomic to Global Scale,"** APS March Meeting 2025, Anaheim, USA (*03/25*).

139 "**Ferrous Iron Partitioning in the Earth's Lower Mantle,"** High-Pressure Gordon Conference 2024, Holderness, USA (*07/24*).

138 (Plenary) "**Modeling Earth from Atomic to Global Scale,"** IUPAP Conference in Computational Physics 2024, Thessaloniki, Greece (*07/24*).

137 "**US-Africa Initiative in Electronic Structure" (together with Richard Martin),** APS March Meeting 2024, Minneapolis, USA (*03/24*).

136 "**Townhall Meeting: A Science Gateway for Mineral and Rock Physics,"** American Geophysical Union Fall Meeting, San Francisco, USA (*12/23*).

135 "**How ESO Tables should be Used by our Community,"** Joint 28th AIRAPT and 60th EHPRG, Edinburgh, Scotland (*07/23*).

134 "**Spin Crossovers in Iron in Lower Mantle Minerals,"** Workshop on Deep Modeling for Molecular Simulations 2023, Princeton, USA (*07/23*).

133 "**Spin Crossovers in Iron in Lower Mantle Minerals,"** ASESMA-2023, Kigali, Rwanda (*06/23*).

132 "**Quasiharmonic Thermodynamics and Thermoelasticity of Lower Mantle Phases,"** ASESMA-2023, Kigali, Rwanda (*06/23*).

131 **"Discovering the Mineralogy of Super-Earth Type Planets,"** American Geophysical Union Fall Meeting, Chicago, USA (*12/22*).

130 **"Thermodynamics of the Iron Spin-Crossover at High-Pressures and Temperatures,"** Workshop on Quantum Thermodynamics, Columbia Global Center, Nairobi, Kenya (*11/22*).

129 **"Ab initio Thermodynamics with the Quasiharmonic Approximation,"** Workshop on Quantum Thermodynamics, Columbia Global Center, Nairobi, Kenya (*11/22*).

131 "**Spin Crossovers in Iron in Lower Mantle Minerals,"** Frontiers of High-Pressure Research – Science Under Extreme Conditions, *Nature Conferences*, Shanghai, China, (*11/22*). (virtual)

127 **"Iron Oxides and Silicates at Extreme Conditions"**, Advanced Quantum ESPRESSO Tutorial: Hubbard and Koopmans Functionals from Linear Response, Lausanne, Switzerland (*11/22*). **(Keynote)** (virtual)

126 **"Modeling the Earth's Mantle from Atomic to Global Scales"**, IUPAP Conference in Computational Physics, Austin, USA (*08/22*). (virtual)

125 **"Modeling the Earth's Mantle from Atomic to Global Scales"**, American Physical Society, Meeting, Chicago, USA (*03/22*).

124 (Plenary) **"Computational Mineral Physics: Challenges and Opportunities"**, Advances in Synchrotron-Based Research - Towards Understanding the Structure, Evolution, and Dynamics of Earth and Planetary Interiors, (Virtual) Meeting, Chicago, USA (*08/21*).

123 (Plenary) **"Spin Crossover in Iron in Lower Mantle Minerals"**, International Conference on Computer Simulation in Physics and Beyond, 2020 Meeting, Moscow, Russia (*10/20*). (virtual)

122 **"Post-PPV transitions in $MgSiO_3$ in Super-Earth's mantles"**, European High Pressure Research Group, 2020 (Virtual) Meeting, Tenerife, Spain (*09/20*). (virtual)

121 **"Ab initio exploration of post-ppv transitions in low pressure analogs of $MgSiO_3$"**, American Chemical Society 2020 Meeting, Philadelphia, USA (*03/20*). (Canceled)

120 **"Spin Crossover in Iron in Lower Mantle Minerals"**, Symposium on Machine Learning in Materials Genome, Spetses, Greece (*07/19*).

119 **"Spin Crossover in Iron in Lower Mantle Minerals"**, AIRAPT 2019, Rio de Janeiro, Brazil (*07/19*).

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

119. **"Quantum phenomena in iron in the mantle and their macroscopic consequences"**, Carnegie-DOE Alliance Center, University of Illinois at Chicago, USA (*12/24*).

118. "**Modeling Earth from atomic to global scale,"** Department of Applied Physics and Applied Mathematics, Columbia University, USA (*10/24*).

117. **"Quantum phenomena in iron in the mantle and their macroscopic consequences"**, Department of Physics Colloquium, Vanderbilt University, USA (*10/24*).

116. **"Iron spin crossover in the Earth's mantle minerals"**, Instituto de Física, Universidade de São Paulo, São Paulo, Brazil (*08/24*).

115. **"Iron partitioning in the Earth's lower mantle: implications for seismic tomography"**, Instituto de Astronomia, Geofísica, e Ciências Atmosféricas, Universidade de São Paulo, São Paulo, Brazil (*08/24*).

114. **"Iron spin crossover in the Earth's mantle and consequences for thermochemical equilibrium"**, Center for Interfacial Science, Department of Chemistry, Princeton University, USA (*03/24*).

113. **"Earth's core related materials problems and simulations"**, Flatiron Institute CCQ, NY, USA (*10/23*).

112. **"Quantum problems in planetary mantle oxides"**, Flatiron Institute CCQ, NY, USA (*09/23*).

111. **"Simulations of Earth and super-Earth's mantle phases: new phases and new physics"**, Laboratório Nacional de Nanotecnologia, CNPEM, Campinas, SP, Brazil (*09/23*).

110. **"Simulations of Earth and super-Earth's mantle phases: new phases and new physics"**, *Quantum Café*, Flatiron Institute CCQ, NY, USA (*05/23*).

109. **"Simulations of Earth and super-Earth's mantle phases: new phases and new physics"**, Colloquium at Lamont-Doherty Earth Observatory, NY, USA (*01/23*).

108. **"Mineralogy of super-Earth's mantles: new phases and new physics"**, Center for Matter at Atomic Pressure, Rochester, USA (*01/23*). (virtual)

107. **"Iron spin crossover's manifestation in the lower mantle"**, Department of Earth Sciences, Princeton, USA (*10/22*). (virtual)

106. **"Spin crossover in iron in lower mantle phases"**, Department of Physics Colloquium, University of Utah (*10/21*). (virtual)

105. **"Spin crossover in iron in lower mantle phases"**, Department of Physics Colloquium, University of Louisiana at Lafayette (*10/21*). (virtual)

104. **"Computational mineral physics: challenges and opportunities",** Centre for Earth Evolution and Dynamics (CEED) and Natural History Museum, University of Oslo, Oslo, Norway (*09/21*). (virtual)

103. **"Emergent views of Earth's lower mantle",** Virtual Research Day: Frontiers in Computational Science and Engineering Research and Software, Columbia University, New York, USA (*05/21*). (virtual)

102. **"Spin crossover in iron in lower mantle phases"**, International Center for Theoretical Physics-East Africa Branch, East-Africa Institute for Advanced Research, Kigali, Rwanda (*02/21*). (virtual)

101. **"High pressure materials research and applications to planetary sciences"**, Department of Physics, University of Texas, El Paso, USA (*10/20*). (virtual)

100. **"Emergent views of Earth's lower mantle"**, Department of Earth and Planetary Sciences, Massachusetts Institute of Technology, Boston, USA (*05/20*). (Canceled and rescheduled for Fall 2021 in person)

99. **"Emergent views of Earth's lower mantle"**, High-Pressure Science and Technology Research (HPSTAR) Center, Beijing, China (*01/20*).

98. **"Spin crossover in iron-bearing minerals of the lower mantle"**, Lawrence Livermore National Laboratory, Livermore, USA (*01/20*).

97. **"Spin Crossover in iron-bearing minerals of the lower mantle"**, Department of Applied Physics and Applied Mathematics, APAM Research Conference Series, Columbia University, New York, USA (*09/19*).

96. **"Emergent views of Earth's lower mantle"**, Geodynamics Seminar Series, Lamont Doherty Earth Observatory, Palisade, NY, USA (*11/19*).

95. **"Cyberinfrastructure for Computational Mineral Physics"**, Computational Science Initiative, Brookhaven National Laboratory, Upton, NY, USA (*07/19*).

94. **"Spin Crossover in Iron in Lower Mantle Minerals"**, Department of Applied Physics and Applied Mathematics, APAM Research Conference Series, Columbia University, New York, USA (*10/18*).

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 or collaborators

84. ***Yang Sun*** - **"*Understanding the stability of superionic phases in Earth's inner core*",** American Geophysical Union Fall'24 Meeting, Washington DC, USA (*12/24*).

83. ***Chenxing Luo*** – **"*Ab initio- based machine-learning studies of ö-AlOOH*",** American Geophysical Union Fall'24 Meeting, Washington DC, USA (*12/24*).

82. ***Yang Sun*** - **"*Crystal structures and motifs in the Fe-Mg-O system under extreme conditions*",** Workshop of Computational Science and Information Engineering, Okinawa, JP (*03/24*).

81. ***Zhen Zhang*** - **"*PBE/GGA predicts the B8-B2 transition in FeO*",** APS March Meeting, Minneapolis, USA (*03/24*).

80. ***Chenxing Luo*** – **"*Elasticity and acoustic velocities of ö-AlOOH*",** American Geophysical Union Fall'23 Meeting, San Francisco, USA (*12/23*).

79. ***Zhen Zhang*** - **"*PBE/GGA predicts the B8-B2 transition in FeO*",** American Geophysical Union Fall'23 Meeting, San Francisco, USA (*12/23*).

78. ***Yang Sun*** - **"*Ab initio* simulations of iron at inner core conditions",** UPAP Conference in Computational Physics, Kyoto, Japan (*08/23*).

77. ***Qi Zhang*** - **"*Ab initio* Thermodynamic and Thermoelasticity Calculations with `Express` Workflows",** Workshop on Computational Quantum Thermodynamics, Columbia Global Center, Nairobi, Kenya (*11/22*).

76. ***Zhen Zhang*** - **"The Phonon Quasiparticle Method",** Workshop on Computational Quantum Thermodynamics, Columbia Global Center, Nairobi, Kenya (*11/22*).

75. ***Chenxing Luo*** - **"*Ab initio* Thermoelasticity Calculations",** Workshop on Computational Quantum Thermodynamics, Columbia Global Center, Nairobi, Kenya (*11/22*).

74. ***Chenxing Luo*** - **"Deep Machine learning potential for atomistic simulation of δ-AlOOH at high pressures and temperatures",** American Geophysical Union Fall'22 Meeting, Chicago, USA (*12/22*).

73. ***Zhen Zhang***- **"Anharmonic thermodynamics and lattice thermal conductivity across the post-perovskite transition in $MgSiO_3$",** American Geophysical Union Fall'22 Meeting, Chicago, USA (*12/22*).

72. ***Yang Sun*** - **"*Ab initio* melting lines of bcc and hcp iron at Earth's inner core conditions",** American Geophysical Union Fall'22 Meeting, Chicago, USA (*12/22*).

71. ***Chenxing Luo*** - **"H-bond disordering in δ-AlOOH",** IUPAP Conference in Computational Physics, Austin, USA (*08/22*).

70. ***Zhen Zhang***- **"Phonon quasiparticle method for calculation of anharmonic properties",** IUPAP Conference in Computational Physics, Austin, USA (*08/22*).

69. ***Yang Sun*** - **"Simulations of iron in the Earth's inner core conditions",** IUPAP Conference in Computational Physics, Austin, USA (*08/22*).

68. ***Yang Sun*** - **"Simulations of iron in the Earth's inner core conditions",** International Workshop on Recent Developments in Electronic Structure, ES'22, New York, USA (*06/22*).

67. ***Yang Sun*** - **"Structure and dynamics of Fe phases under Earth's core conditions",** American Physical Society, March Meeting'22, Chicago, USA (*03/22*).

66. ***Yang Sun*** - **"Fe-rich Fe-O compounds at earth's core pressures",** American Geophysical Union Fall'21 Meeting, New Orleans, USA (*12/21*).

65. ***Zhen Zhang*** - **"Phonon quasiparticle method for calculation of anharmonic properties",** International Center for Theoretical Physics-East Africa Branch, East-Africa Institute for Advanced Research, Kigali, Rwanda (*06/21*). (virtual).

64. ***Zhen Zhang*** - **"Thermal conductivity of cubic $CaSiO_3$-perovskite",** American Physical Society March Meeting'21, (virtual) USA (*03/21*).

63. ***Koichiro Umemoto*** - **"Order-Disorder Transition in Mg2GeO4 at ultra-high pressures",** American Geophysical Union Fall 2020 Meeting, (virtual) USA (*12/20*).

62. ***Grace Sheppard***- **"Seismic detection of the iron spin transition in Earth's lower mantle",** American Geophysical Union Fall 2020 Meeting, (virtual) USA (*12/20*).

61. ***Zhongqing Wu***- **"Velocity and density characteristics of subducted oceanic crust and the origin of seismic heterogeneities in the lower mantle",** American Geophysical Union Fall 2020 Meeting, (virtual) USA (*12/20*).

60. ***Zhen Zhang*** - **"Thermal conductivity of cubic $CaSiO_3$-perovskite",** American Geophysical Union Fall 2019 Meeting, San Francisco, USA (*12/19*).

59. ***Arie van den Berg*** - **"Mass-dependent Dynamics of Terrestrial Exoplanets Using ab initio Mineral Properties"**, American Physical Society 2019 March Meeting, Boston, USA (*03/19*).

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*).