RENATA M. M. WENTZCOVITCH
Professor of Applied Physics and Materials Science
Department of Applied Physics and Applied Mathematics
Department of Earth and Environmental Sciences
Lamont-Doherty Earth Observatory
Columbia University
rmw2150@columbia.edu
http://www.mineralscloud.com/

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

Israa Draz (06/2025-) Undergraduate Summer Intern, Lamont Doherty Earth Observatory.

Jose Maria Osa (06-08/2025) Undergraduate Summer Intern, Lamont Doherty Earth Observatory.

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-) Postdoc 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 Kark*i (*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, a 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, Postdoc 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 a postdoc at the Department of Chemical Engineering and TAC, U. of Texas-Austin.

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. Currently, PhD student in Materials Science, Stanford University.

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, a Postdoctoral Fellow at Lamont-Doherty Earth Observatory, Columbia University.

4. Alumni: Undergraduate

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

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

• Bridgman Award of the International Association for Advancement of Research in High Pressure Science and Technology (*2025*) (*first woman*)
• 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) Organizer, Town Hall Meeting, *A Science Gateway for Mineral and Rock Physics*, American Geophysical Union Fall Meeting, San Francisco, USA *(12/2023).*

4) 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).*

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, Chicago, USA *(12/2022).*

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; 2025)*

-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*, the news magazine of the American Geophysical Union (*2025-prsent)*

- 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)*