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

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

B. EDUCATION

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

C. PROFESSIONAL EXPERIENCE

1. Columbia University

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

2. University of Minnesota

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

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

2. Post-doctoral Appointments

• Research Fellow, Department of Geological Sciences, University College London, and The Royal Institution of Great Britain, London, UK, with David G. Price, *(1993-94)*

• Theory of Condensed Matter Group (TCM), Cavendish Laboratory, Cambridge, UK, with Volker Heine *(1992-93)*
• Department of Physics, Brookhaven National Laboratory, and Department of Physics, Stony Brook University, with Philip B Allen *(1989-92)*

3. Affiliations with Other Institutions

• Adjunct Research Scientist, Lamont Doherty Earth Observatory, Columbia University (*08/2016*-)
• Principle Investigator at the Earth-Life Science Institute (ELSI), World Premier International Research Institute (WPIRI) of the JSPS, Tokyo Institute of Technology, Tokyo, Japan *(10/2012-2016).* Associate Investigator (*2017*-)
• Visiting Professor, Computational Science Research Center, Chinese Academy of Engineering Physics, Beijing, China *(06/2015, 10-11/2016).*
• Visiting Professor, Department of Earth and Space Sciences, University of Science and Technology of China, Hefei, China *(07/2012, 8/2013).*
• Visiting Professor, Faculty of Sciences, Interactive Center for Science, Tokyo Institute of Technology, Tokyo, Japan *(5/2010-8/2010)*
• Visiting Professor, Departments of Physics and Earth and Planetary Sciences, Tokyo Institute of Technology, Tokyo, Japan *(04/2002, 08/2006, 10-12/2008)*
• Visiting Professor, Departments of Geology, University of Frankfurt, Germany *(09/2008-11/2008, 08/2009, 08/2010, 08/2012)*
• Visiting Professor Department of Physics and Astronomy and Department of Geological Sciences, (*Fall* 2005) and Department of Physics and Astronomy *(08/1995, 02/1996, 08/1997, 07/1998)*, Stony Brook University, Stony Brook, NY, USA .
• Distinguished Visiting Professor (*2005*), Visiting Professor *(08/2001, 08/2002, 08/2003, 08/2004, 08/2012, 08/2017)* and Visiting Scientist *(08/1998, 08/1999, 08/2000)*, Scuola Internazionale Superiori di Studi Avanzati, SISSA, Trieste, Italy
• Visiting Scientist, National Institute for Computer Science and Engineering, INESC, Lisbon, Portugal, *(01/1996)*
• Assistant Professor, Department of Materials Physics, Institute of Physics, University of São Paulo, Brazil *(1995-96)*
• Visiting Researcher, The James Franck Institute, University of Chicago *(Fall 1988)*

D. HONORS AND AWARDS

• Wilhelm Heraeus Visiting Professorship Award, University of Frankfurt (€40,000) (*2015-16*)
• Fellow, American Academy of Arts and Sciences (*2013*-)
• Fellow, American Association for Advancement of Science (Physics) (*2012*-)
• Fellow, Mineralogical Society of America (*2009*-)
• Fellow, American Geophysical Union (*2008*-)
• Fellow, American Physical Society, Division of Materials Physics (*2006*-)
• Alexander von Humboldt Research Award for Senior US Scientists (€60,000) (*2008*)
• Japan Society for Progress of Science (JSPS), Invitation Fellowship for Research in Japan (*2008*)

• Member at-large, American Physical Society, Division of Computational Physics (*2000-03*)
• Fellow (*2001-*) and Associate Fellow (*1997-2001*) of Minnesota Supercomputing Institute
• 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.
• 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)

E. PERSONNEL SUPERVISION

• *Current Advisees*

Columbia University

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

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

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

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

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

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

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

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

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

University of Minnesota

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

• *Alumni: Post-doctoral fellows*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

• <u>*Alumni: Graduate students*</u>

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

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

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

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

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

Pedro da Silveira (PhD graduate student, Scientific Computing *2008-14*). Currently, senior software engineer, Digital River, Minnetonka, MN.

Gaurav Shukla (PhD, Physics, *2011-15*) Assistant Professor of Physics, Bennet University, New Delhi, India.

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

• <u>*Alumni: Undergraduate students*</u>

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

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

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

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

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

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

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

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

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

• *Alumni: Visiting students and researchers*

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

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

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

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

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

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

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

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

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

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

1) Program Chair of the Division of Computational Physics, APS March Meeting 2019, Boston. 120+ sessions.

2) 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.

3) 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 *(2017).*

4) 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*).

5) 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*).

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

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

8) 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).*

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

10) 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).*

11) 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).*

12) 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).*

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

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

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

16) 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).*

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

18) 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).*

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

20) 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.

21) 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).*

22) 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).*

23) 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).*

24) 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*).

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

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

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

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

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

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

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

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

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

34) 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).*

35) 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*).

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

G. PUBLICATIONS

2018

195. K. Sarkar, N. Holzarth, and R. M. Wentzcovitch, **EPAW-1.0 code for evolutionary optimization of PAW datasets especially for high-pressure application**, *Comp. Phys. Comm.*, in press (2018). DOI:10.1016/j.cpc.2018.05.019

194. H. Yun, M. Topsakal, A. Prakash, K. Ganguly, C. Leighton, B. Jalan, R. M. Wentzcovitch, J. S. Jeong, and K. A. Mkhoyan, **Electronic structure of $BaSnO_3$ investigated by high energy resolution EELS and *ab initio* calculations**, *J. Vac. Sci. Technol. A* **36**, 031503 (2018). DOI: 10.1116/1.5026298 **Featured article**.

193. T. Qin, R. M. Wentzcovitch, K. Umemoto, M. Hirschmann, and D. Kohlstedt, ***Ab initio* study of water speciation in forsterite: importance of the entropic effect**, *American Mineralogist*, in press (2018). DOI: 10.2138/am-2018-6262

192. M. L. Marcondes, R. M. Wentzcovitch, L. V. C. Assali, **Importance of Van der Waals interaction on structural, vibrational, and thermodynamics properties of NaCl**, *Solid State Comm.* **273**, 11-16 (2018) DOI: 10.1016/j.ssc.2018.01.008

2017

191. J. Valencia-Cardona, Q. Williams, G. Shukla, and R. Wentzcovitch, **Bullen's parameter as a seismic observable for spin crossover in the lower mantle,** *Geophys. Res. Lett*. **44**, 9314 (2017). DOI: 10.1002/2017GL074666

190. D.-B. Zhang, P. B. Allen, T. Sun, and R. M. Wentzcovitch, **Sub-minimum mean free path in $MgSiO_3$-perovskite: insights from phonon quasiparticles,** *Phys. Rev. B* **96**, 100302(R) (2017). DOI: 10.1103/PhysRevB.96.100302

189. K. Umemoto, R. M Wentzcovitch, S. Q. Wu, M. Ji, C. Z. Wang, K.-M. Ho, **Phase transitions in $MgSiO_3$ post-perovskite in terrestrial exoplanetary mantles**, *Earth and Planet. Sc. Lett.* **478**, 40 (2017). DOI: 10.1016/j.epsl.2017.08.032

188. N. Ghaderi, D.-B. Zhang, H. Zhang, J. Xian, T. Sun, and R. M. Wentzcovitch, **Lattice thermal conductivity of $MgSiO_3$ perovskite from first principles,** *Scient. Rep.* **7**, 5417 (2017). DOI:10.1038/s41598-017-05523-6

187. K. Sarkar, M. Topsakal, N. Holzwarth, and R. M. Wentzcovitch, **Evolutionary optimization of PAW data-sets for high-pressure simulations**, *J. Comp. Phys.* **347**, 39 (2017). DOI: 10.1016/j.jcp.2017.06.032

186. J. Valencia-Cardona, G. Shukla, Z. Wu, D. Yuen, C. Hernlund, and R. Wentzcovitch, **Effect of the iron spin crossover in ferropericlase on the mantle geotherm**, *Geophys. Res. Lett*. **44**, 4863 (2017). DOI: 10.1002/2017GL073294

185. K. Umemoto and R. Wentzcovich, **Theoretical study of the volume isotope effect in H_2O ice**, *Jap. J. Appl. Phys.* **56**, 05FA03 (2017). DOI:10.7567/JJAP.56.05FA03

184. Y. Lu, T. Sun, P. Zhang, P. Zhang, D.-B. Zhang, and R. M. Wentzcovitch, **Pre-melting bcc to hcp transition in beryllium**, *Phys. Rev. Lett*. **118**, 145702 (2017). DOI: 10.1103/PhysRevLett.118.145702

183. M. Ballmer, C. Houser, J. Hernlund, R. M. Wentzcovitch, and K. Hirose, **Persistence of strong silica-enriched domains in the Earth's lower mantle**, *Nature Geoscience* **10**, 236 (2017). DOI: 10.1038/NGEO2898

182. Z. Wu and R. Wentzcovitch, **Composition versus temperature induced velocity heterogeneities in a pyrolytic lower mantle**, *Earth and Planet. Sc. Lett.* **457**, 359–365 (2017). DOI: 10.1016/j.epsl.2016.10.009

2016

181. G. Shukla and R. M. Wentzcovitch, **Spin crossover in $(Mg,Fe^{3+})(Si,Fe^{3+})O_3$ bridgmanite: effects of disorder, iron concentration, and temperature**, *Phys. Earth and Planet. Int.* **50**, 53-61 (2016). DOI: 10.1016/j.pepi.2016.09.003

180 J. S. Jeong, M. Topsakal, P. Xu, B. Jalan, R. M. Wentzcovitch, and A. Mkhoyan, **A new line defect in strained $NdTiO_3$ perovskite**, *Nano-Letters* **16**, 6816-6822 (2016). DOI: 10.1021/acs.nanolett.6b02532

179. M. Topsakal, C. Leighton, and R. Wentzcovitch, **Electronic and structural properties of *Re*CoO_3 investigated using DFT+U**, *J. Appl. Phys.* **119**, 244310 (2016). DOI: 10.1063/1.4954792

178. K. Umemoto, T. Kawamura, K. Hirose, and R. M. Wentzcovitch, **Post-stishovite transition in hydrous aluminous SiO_2**, *Phys. Earth & Planet. Int.* **255**, 18-26 (2016). DOI:10.1016/j.pepi.2016.03.008

177. G. Shukla, M. Cococcioni, and R. Wentzcovitch, **Thermoelasticity of Fe^{3+}- and Al-bearing bridgmanite: effects of spin crossover in iron**, *Geophys. Res. Lett.* **43**, 5661–5670 (2016). DOI: 10.1002/2016GL069332s

2015

176. M. M. Lacerda, G. Shukla, and R. M. Wentzcovitch, **Accurate thermoelastic tensor and acoustic velocities of NaCl**, *AIP-Advances* **5**, 127222 (2015). DOI:10.1063/1.4938550

175. K. Umemoto, E., Sugimura, K. Hirose, S. de Gironcoli, and R. M. Wentzcovitch, **Nature of the volume isotope effect in H_2O-ice**, *Phys. Rev. Lett.* **115**, 173005 (2015). DOI:10.1103/PhysRevLett.115.173005

174 G. Shukla, M. Topsakal, and R. Wentzcovitch, **Spin crossovers in iron-bearing $MgSiO_3$ and $MgGeO_3$: their influence on the post-perovskite transitions**, *Phys. Earth & Planet. Int.* **249**, 11-27 (2015). DOI:10.1016/j.pepi.2015.10.002

173. R. Wu, M. Topsakal, M. Robbins, N. Haratipour, J. Jeong, R. Wentzcovitch, S. Koester, and K. A. Mkhoyan, **The Atomic and Electronic Structure of Exfoliated Black Phosphorus**, *J Vac Sc Tech A* **33**, 060604 (2015). DOI:10.1116/1.4926753

172. K. Umemoto, B. Himmetoglu, J. P. Wang, R. Wentzcovitch, and M. Cococcioni, **Searching for high magnetization density in bulk Fe: the new metastable Fe_6 phase**, *J. Phys.: Cond. Matt.* **27**, 016001 (2015). DOI:10.1088/0953-8984/27/1/016001

171. K. Hirose, T. Lay, R. M. Wentzcovitch, and D. A. Yuen, **Mineralogy of the deep mantle – the post-perovskite phase and its geophysical significance**, *Treatise in Geophysics* **2**, 85-115 (2015). DOI:10.1016/B978-0-444-53802-4.00054-3

170. M. M. Lacerda and R. M. Wentzcovitch, **Hybrid *ab-initio*/experimental high temperature equations of state: the NaCl pressure scale**, *J. Appl. Phys.* **117**, 215902 (2015). http://dx.doi.org/10.1063/1.4921904

169. G. Shukla, Z. Wu, H. Hsu, A. Floris, M. Cococcioni, and R. Wentzcovitch, **Thermoelasticity of (Mg,Fe)SiO_3 perovskite**, *Geophys. Res. Lett.* **42**, 1749 (2015). DOI:10.1002/2014GL062888

2014

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4. VIDEO

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