RENATA M. M. WENTZCOVITCH
Department of Applied Physics and Applied Mathematics,
Department of Earth and Environmental Sciences, Lamont Doherty Earth Observatory,
Columbia University, New York, NY, U.S.A.

HISTORY OF EMPLOYMENT

Professor, Department of Applied Physics and Applied Mathematics,
Fu Foundation School of Engineering, Columbia University, 2017-present

Professor, Department of Earth and Environmental Sciences,
Lamont Doherty Earth Observatory, Columbia University, 2017-present

Professor of Materials Science and Engineering, U. of Minnesota, 2006-2016

Associate Professor of Materials Science, U. of Minnesota, 2001-2006

Assistant Professor of Materials Science, U. of Minnesota, 1994-2001

Research Fellow, Department of Geological Sciences, University College London and The Royal Institution of Great Britain, London, UK, 1993-1994

Post-doctoral Researcher at the Theory of Condensed Matter Group (TCM), Cavendish Laboratory, Cambridge, UK, 1992-1993

Post-doctoral Researcher in the Department of Physics, Brookhaven National Laboratory, and Department of Physics, Stony Brook U., 1989-1992

DEGREES

U. of São Paulo	São Paulo, Brazil	Physics	B.A., 1980
U. of São Paulo	São Paulo, Brazil	Physics	M.Sc., 1982
U. of California-Berkeley	Berkeley, CA	Physics	Ph.D., 1988

RESEARCH EXPERIENCE

I am a computational materials physicist who developed *ab initio* simulation methods to investigate materials at extreme conditions of temperature and pressure. The first of these methods is referred to as Born-Oppenheimer molecular dynamics (BOMD) and is broadly used in materials simulations. In 1992, when looking for the most interesting problems to apply this method, I came across $MgSiO_3$-perovskite (bridgmanite), whose behavior at lower mantle (LM) pressures was still unknown. That problem introduced me to mineral physics and geophysics to which I have contributed since. Other key methodological developments motivated by mineral physics include *ab initio* thermodynamics with the quasiharmonic approximation, thermoelasticity, anharmonic thermodynamics and thermal conductivity with phonon quasiparticles, and an adaptive genetic algorithm for material discovery. I also introduced a theory for the spin crossover in iron in LM phases. These methods combined have been widely applied to minerals providing data for interpretation of seismic tomographic images and input for more realistic geodynamics simulations. Seismology, geodynamics, and mineral physics are today integrated into a cohesive simulation field, planetary interior modeling. In short, I have assisted in the introduction of materials simulations in geophysics.

HONORS AND AWARDS

Vice-Chair, Chair-Elect, Chair, Past-Chair, Division of Computational Physics, American Physical Society (*2017-21*)

Outstanding Referee for Physical Review Journals (*2022*)

Wilhelm Heraeus Visiting Professorship Award, University of Frankfurt (*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 (*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 (*2000-02*)
Fellow (*2001-2016*) and Associate Fellow (*1997-2001*) of Minnesota Supercomputing Institute
Shell Land-Grant Professor in 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 research, *1978-80*), National Council for Nuclear Energy, CNEN (M.Sc., *1980-82*), National Research Council, CNPq (Ph.D. at UC-Berkeley, *1983-87*)

SELECTED PUBLICATIONS

1. *Ab initio* molecular dynamics with variable cell shape: application to $MgSiO_3$, **R. Wentzcovitch,** J. L. Martins, and G. D. Price, *Phys. Rev. Lett.* 70, 3947 (1993).
2. Polymorphs of alumina predicted by first principles: putting pressure on the ruby pressure scale, K. Thomson, **R. M. Wentzcovitch**, and M. S. T. Bukowinski, *Science* 274, 1880 (1996).
3. First-principles determination elastic anisotropy and wave velocities of MgO at lower mantle conditions, B. B. Karki, **R. M. Wentzcovitch**, S. de Gironcoli, and S. Baroni, *Science* 286, 1705 (1999).
4. Thermoelastic properties of of $MgSiO_3$-perovskite: insights on the nature of the Earth's lower mantle, **R. Wentzcovitch**, B. B. Karki, M. Cococcioni, and S. de Gironcoli, *Phys. Rev. Lett.* 92, 018501 (2004).
5. Phase Transition in $MgSiO_3$-perovskite in the Earth's Lower Mantle, T. Tsuchiya, J. Tsuchiya, K. Umemoto, and **R. Wentzcovitch**, *Earth Planet. Sci. Lett.* 224, 241 (2004).
6. $MgSiO_3$ post-perovskite at D″ conditions, **R. Wentzcovitch**, T. Tsuchiya, J. Tsuchiya, *Proc. Natl. Acad. Sc.* 103, 543 (2006).
7. Spin transition in Magnesiowüstite in Earth's lower mantle, T. Tsuchiya, **R. Wentzcovitch,** C. R. S. da Silva, S. de Gironcoli, , *Phys, Rev, Lett.* 96, 198501 (2006).
8. Dissociation of $MgSiO_3$ in the Cores of Gas Giants and Terrestrial Exoplanets, K. Umemoto, **R. Wentzcovitch**, and P. B. Allen, *Science* 311, 983 (2006).
9. Anomalous compressibility of ferropericlase throughout the iron spin crossover, **R. Wentzcovitch**, J. F. Justo, Z. Wu, C. R. S. da Silva, D. Yuen, and D. Kohlstedt, *Proc. Natl. Acad. Sc. USA* 106, 8447 (2009).
10. Elastic anomalies in a spin-crossover system: ferropericlase at lower mantle conditions, Z. Wu, J. F. Justo, and R. M. Wentzcovitch, *Phys. Rev. Lett.* **110**, 228501 (2013).
11. Spin crossover in ferropericlase and velocity heterogeneities in the lower mantle, Z. Wu and **R. Wentzcovitch**, *Proc. Natl. Acad. USA* 111, 10468 (2014).
12. Persistence of strong silica-enriched domains in the Earth's lower mantle, M. D. Ballmer, C. Houser, J. Hernlund, **R. M. Wentzcovitch**, and K. Hirose, *Nature Geoscience* 10, 236 (2017).
13. Velocity and density characteristics of subducted oceanic crust and the origin of seismic heterogeneities in the lower mantle, W. Wang, Y. Xu, D. Sun, S. Ni, **R. M. Wentzcovitch**, and Z. Wu, *Nature Communications* 11, 1 (2020).
14. Seismic detection of the iron spin transition in Earth's lower mantle, G. Shephard, C. Houser, J. Hernlund, J. Valencia-Cardona, R. Trönne, and **R. Wentzcovitch**, *Nature Communications* 12, 5905 (2021).
15. Two-step nucleation of the Earth's inner core, Y. Sun, F. Zhang, M. Y. Mendelev, **R. M. Wentzcovitch**, K.-M. Ho, *Proc. Natl. Acad. USA* 119, e2113059199(2022).

SOCIETY MEMBERSHIPS

American Geophysical Union, American Physical Society, Mineralogical Society of America, American Association of the Advancement of Science, American Academy of Arts and Sciences.