

Ronald E. Cohen

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My research uses first-principles methods to understand, predict properties, and design materials. I have a classical background in geology, but have studied and applied computational physics extensively to the understanding of Earth and technological materials. I work closely with experimentalists to design and understand experiments, with geophysicists and geochemists to understand Earth structure and behaviour, and with material scientists, physicists, and chemists to understand materials.

Born March 5, 1957 Lafayette, IN, USA

Professional Preparation:

Oberlin College		1975-1976
Indiana University	Geology	B.S., 1979
Harvard University	Geology	A.M., 1981
Harvard University	Geology	Ph.D., 1979-1985

Thesis: *Thermodynamics of Aluminous Pyroxenes: Effects of Short-Range Order*

Appointments:

2015-: Visiting Professor, Department for Earth and Environmental Sciences,
LMU, Munich

2015-: Honorary Professor, Department of Physics, University College London,
Gower Street, London, WC1E 6BT, UK

2013-2015: Honorary Professor, London Centre for Nanotechnology,
University College London, Gower Street, London, WC1E 6BT, UK

2013-2015: Professor, Department of Earth Science, University College London,
Gower Street, London, WC1E 6BT, UK

1990-: Senior Staff Member, Geophysical Laboratory

2000-2001: Visiting Professor, Materials Science and Geophysics, California Institute
of Technology

1988-1990: Visiting Investigator, Geophysical Laboratory

1987-1990: Research Physicist, Naval Research Laboratory

1985-1987: Research Associate, National Research Council, NRL

Publications and invited talks:

215 papers published, 229 invited talks, h-index: 59, 66 citations/paper, 28 papers with over 100 citations

Most cited paper: Cohen, R.E., Origin of ferroelectricity in oxide ferroelectrics. Nature 1992. 358: p. 136-138, citations: 1658.

Synergistic Activities and Professional Service:

Developed and fostered field of theory of ferroelectrics by a series of annual workshops beginning in 1990

Contributed in development of public codes and methods used to simulate materials at the atomic scale

Edited High-Performance Computing Requirements for the Computational Solid Earth Sciences, 96 pp, http://www.geo-prose.com/computational_SES.html (2005).

Served as chair and serves as member of Mineral and Rock Physics Committee of AGU

Honors and Memberships in Professional Societies:

Dana Medal, Mineralogical Society of America, 2009, Fellow of American Physical Society, 2002, Fellow of American Geophysical Union, 2002, Doornbos Memorial Prize from International Association of Seismology and Physics of the Earth's Interior (IASPEI), 1994, Mineralogical Society of America Award and Life Fellow, 1994, Berman Research Publication Award, NRL, 1993, IBM Supercomputing Competition, Second Prize in Science, 1990, Berman Research Publication Award, NRL, 1988, National Research Council, Research Associateship, 8/85-8/87, National Science Foundation Graduate Fellowship, 9/79-8/82, Member, American Association for the Advancement of Science, Member, Member, Geological Society of America, Member, Phi Beta Kappa, Sigma Xi

Recent Collaborators: M. Ahart (GL), B. Burton (NIST), R. Caracas (CNRS – ENS Lyon), E. Cockayne (NIST), P. Dera (APS), K. Driver (Ohio State), A. Goncharov (GL), E. Gregoryanz (U. Edinburgh), C. Guillaume (U. Edinburgh), K. Haule (Rutgers), R. J. Hemley (GL), Jeongnim Kim (NCSA), G. Kotliar (Rutgers), A. Lazicki (LLNL), Peter Liermann (GL), Z. Liu (GL), B. Militzer (UC Berkeley), R. Ren (APS), P. Lopez Rios (Univ. Cambridge), H.K. Mao (GL), A. Millis (Columbia), R. Needs (Univ. Cambridge), S. Savrasov (UC Davis), M. Somayazulu (GL), V. Struzhkin (GL), M. Towler (Univ. Cambridge), J.W. Wilkins (Ohio State), Z. Wu (CSM), W. Yang (APS), Z.-G. Ye (Simon-Fraser)

Graduate, Post-doctoral Advisors and Supervisors: L. L. Boyer (NRL, retired), C. W. Burnham, Jr. (Harvard, Emeritus), J. F. Hays (Harvard, Emeritus), R.J. Hemley (GL), W. Huntress (GL), B. Klein (UC Davis), D. Papaconstantopolous (George Mason Univ.), C. T. Prewitt (Univ. Ariz), J. B. Thompson (Harvard, deceased), J. A. Wood (Harvard, Emeritus)

Supervised Students, Post-doctoral Fellows, and Research Associates: R. Caracas (Lyon), N. Choudhury (UA), K. Esler (UIUC), H. Fu (Univ. Ark.), P. Ganesh (ORNL), O. Gulseren (Turkey), I. Inbar (classified), D. Isaak (UCLA/Azusa), J. Ita (Shell Oil), F. Marton (Bergen Community College), X. Luo, I. Mazin (NRL), S. Mukherjee (Seagate), M. Rose (U. Chicago), X. Sha (GMU), L. Shulenburg (SNL), G. Steinle-Neumann (BGI), Q. Peng (Zhejiang Normal University, China), L. Stixrude (UCL), J. Weitz (Ga. Tech.), Z. Wu (Colorado School of Mines)

Funding profile (partial)

Theory of Core Mantle and Technological Materials (ToMcaT), European Research Council Advanced Grant, 2,650,047 Euro, 10/2013-9/2016

First-principles Theory and Fundamental Experiments on New Transducer Materials, ONR N00014-14-1-0561 \$500,000, 6/1/14-5/30/17

CMG Collaborative Research: Quantum Monte Carlo Calculations of Deep Earth Materials, Ronald Cohen, NSF \$189,997, 1/01/11 - 07/30/13

First Principles Calculations of Physical Properties and Bonding in Ferroelectrics, Ronald Cohen, ONR N00014-07-1-0451, \$420,402, 12/20/2009-12/31/2016

Theoretical Investigations of Mantle and Core Materials, Ronald Cohen, NSF EAR-1214807, \$326,000, 01/1/2012-6/30/2016

Theoretical Investigations of Mantle and Core Materials, Ronald Cohen, NSF EAR-0738061

(02095), \$254,000, 01/17/2008-1/31/2010

CMG Collaborative Research: Quantum Monte Carlo Calculations for Deep Earth Materials, Ronald Cohen EAR-0530282, \$575,000, 09/15/2005-08/31/2010

Aspen Center for Physics Winter Conference on Advances in the Fundamental Physics of Ferroelectrics and Related Materials, Ronald Cohen, NSF GRANT10417583, \$25,000, 1 October 2009-30 September 2010

Collaborative Research: CMG: Quantum Monte Carlo Calculations of Deep Earth Materials, Ronald Cohen, NSF EAR-0530282, \$575,000, 09/15/05 - 08/31/09

First-Principles Calculations of Physical Properties and Bonding in Ferroelectrics, Ronald Cohen, ONR N00014-07-1-0451, \$265,040.00, 12/20/2006-12/31/2009

A Facility for Simulating the Dynamic Response of Materials, subcontract from Caltech from ASC DOE, Californian Institute of Technology to Geophys. Lab., \$936,771 09/01/97 - 08/30/07

Theoretical investigations of mantle minerals, Ronald Cohen, NSF, \$300,000, 07/01/03 - 07/30/06

First-Principles Calculations of Physical Properties and Bonding in Ferroelectrics. ONR N00014-92-J-1019(2) 1,316,184 09/01/96 - 12/31/06

Collaborative Project: Theoretical Investigation of Core Materials from First-Principles: Solid and Liquid Phases and Melting on Iron. NSF EAR \$90,000; 5/01/00-4/30/04

Ten most cited publications published in last ten years h-index 59

Wu, Z. G. & Cohen, R. E. More Accurate Generalized Gradient Approximation for Solids. *Physical Review B* 73, doi:235116 10.1103/PhysRevB.73.235116 (2006). Citations: 828.

Ahart, M., Somayazulu, M., Cohen, R. E., Ganesh, P., Dera, P., Mao, H. K., Hemley, R. J., Ren, Y., Liermann, P. & Wu, Z. G. Origin of Morphotropic Phase Boundaries in Ferroelectrics. *Nature* 451, 545-U542, doi:10.1038/nature06459 (2008). Citations: 308.

Wu, Z. G. & Cohen, R. E. Pressure-Induced Anomalous Phase Transitions and Colossal Enhancement of Piezoelectricity in PbTiO₃. *Physical Review Letters* 95, doi:037601 10.1103/PhysRevLett.95.037601 (2005). Citations: 220.

Xiao-Jia Chen, Viktor V Struzhkin, Zhigang Wu, Maddury Somayazulu, Jiang Qian, Simon Kung, Axel Nørnlund Christensen, Yusheng Zhao, Ronald E Cohen, Ho-kwang Mao, Russell J Hemley, Hard superconducting nitrides, *Proceedings of the National Academy of Sciences*, 102, 3198-3201 (2005) Citations: 158.

Wu, Z. G., Chen, X. J., Struzhkin, V. V. & Cohen, R. E. Trends in Elasticity and Electronic Structure of Transition-Metal Nitrides and Carbides from First Principles. *Physical Review B* 71, doi:214103 10.1103/PhysRevB.71.214103 (2005). Citations: 131.

Caracas, R. & Cohen, R. E. Effect of Chemistry on the Stability and Elasticity of the Perovskite and Post-Perovskite Phases in the MgSiO₃-FeSiO₃-Al₂O₃ System and Implications for the Lowermost Mantle. *Geophysical Research Letters* 32, doi:L16310 10.1029/2005gl023164 (2005). Citations: 86.

Mao, W. L., Meng, Y., Shen, G. Y., Prakapenka, V. B., Campbell, A. J., Heinz, D. L., Shu, J. F., Caracas, R., Cohen, R. E., Fei, Y. W., Hemley, R. J. & Mao, H. K. Iron-Rich Silicates in the Earth's D " Layer. *Proceedings of the National Academy of Sciences of the United States*

of America 102, 9751-9753, doi:10.1073/pnas.0503737102 (2005). Citations: 74.

Sha, X and R.E. Cohen, Lattice dynamics and thermodynamics of bcc iron under pressure: First-principles linear response study, *Physical Review B*, 73, 104303 (2006). Citations: 59

Caracas, R. and R.E. Cohen, Prediction of a new phase transition in Al₂O₃ at high pressures,, *Geophysical Research Letters* 32 (6) (2005). Citations: 46

R.E. Cohen, Relaxors go critical, *Nature* 441 (7096), 941-942 (2006). Citations: 42

Patents

U.S. Patent No. 8,039,131 B2 October 18, 2011 Class of pure piezoelectric materials

U.S. Patent No. 8,287,831 October 16, 2012 Oxynitride Perovskites

U. S Patent No. 8,721,915 B2 May 2014 Ordered Oxynitride Perovskites

Sample of Invited Talks at International Meetings (out of about 80 invited talks during period)

1. Polarization Rotation in Relaxor Ferroelectrics, 12th US-Japan Seminar on Dielectric and Piezoelectric Ceramics, November 6–9, 2005, Marriott Waterfront Hotel, Annapolis, Maryland.
2. Polarization Rotation and Domain Contributions to Large Electromechanical Coupling in Relaxor Ferroelectrics, 11th International Meeting on Ferroelectricity, IMF11, Iguassu Falls Brazil/Argentina, September 4-9, 2005.
3. Theory of Iron at High Pressure and Temperature, Workshop on Synergy of 21st Century High-Pressure Science and Technology, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois USA, May 1, 2006.
4. Origin of Large Response in High Electromechanical Coupling Transducer Materials, 2006 U.S. Navy Workshop on Acoustic Transduction Materials and Devices, Penn. State University, State College, PA, May 9, 2006.
5. Theory of Iron at High Pressure and Temperature, Conference on Mathematical Geophysics, Sea of Gallilee, Israel, June 4-8, 2006.
6. Theory of Iron at High Pressure and Temperature, CECAM workshop on Mineral Physics with Computation and Experiment, Lyon, France, June 19-23, 2006.
7. Origin of large response in high electromechanical coupling transducer materials, COE21, Waseda University, Tokyo, Japan, Sept. 6, 2006.
8. Enhanced Piezoelectricity from Polarization Rotation in Perovskites, APS March meeting, Denver, CO, March 5, 2007.
9. Theory of Minerals at High Pressures Beyond Band Theory, SMEC 2007 - Study of Matter at Extreme Conditions, Miami Beach, Miami Beach, April 18, 2007, Plenary Talk.
10. Quantum Monte Carlo and Dynamical Mean Field Theory for solids at high pressures, Electronic Structure Workshop, June 14, 2007, NCSU, NC, USA.
11. Polarization rotation in large strain piezoelectrics and new polar materials by design, European Meeting on Ferroelectricity, Sept. 5, 2007, Bled, Slovenia.
12. Joint Theoretical and Experimental Studies for Developing New Transducer Materials, 2008 U.S. Navy Workshop on Acoustic Transduction Materials and Devices, Penn Stater, Conference Center Hotel in State College, Pennsylvania, May 13 – 15, 2008.
13. Overview of Deep Carbon Reservoirs, Keynote Talk, Deep Carbon Cycle Workshop, Geophysical Laboratory, Broad Branch Road Campus, Washington, D.C., May 15-17, 2008.
14. Joint Theoretical and Experimental Studies for Developing New Electromechanical Materials, High Pressure Workshop, NSLS, May 21, 2008.
15. Joint Theoretical and Experimental Studies for Developing New Electromechanical Materials, 2nd International Conference on Quantum Simulators and Design (QSD2008) to be held in the National Museum of Emerging Science and Innovation (Miraikan), Tokyo, Japan, May 31-June 3, 2008.
16. Theoretical and experimental studies of ferroelectrics and relaxors under pressure,

- Japanese Physical Society, Morioka, Japan, Sept. 21, 2008.
17. Melting at High Pressures, American Geophysical Union, San Francisco, Dec. 2008.
 18. Quantum Monte Carlo Computations for Minerals at High Pressures, San Francisco, Dec. 2008.
 19. Quantum Monte Carlo Simulations of Behavior of Materials at Extreme Conditions, 14th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, ICTP, Trieste, IT, Jan. 8, 2009.
 20. Theoretical Studies for Developing New Electromechanical Materials, Fundamental Physics of Ferroelectrics 2009, Williamsburg, VA, Feb. 2009.
 21. Transducer Materials by Design, 2009 U.S. Navy Workshop, Penn State, May 14, 2009.
 22. New directions in accurate predictions of high pressure mineral properties, Interior of the Earth Gordon Research Conference, Mount Holyoak, MA, June 16, 2009.
 23. Properties of minerals and other things from fundamental physics: From DFT to DMFT and QMC, Goldschmidt Conference, Davos, Switzerland, June 24, 2009.
 24. Quantum Monte Carlo Simulations of Materials under Extreme Conditions, AIRAPT, Tokyo, Japan, July 28, 2009.
 25. First-principles and Experimental Studies on Ferroelectrics and Relaxors, MRS, Boston, Dec. 3, 2009.
 26. Elastic isotropy of iron under core conditions and other recent advances, R.E. Cohen and X. Sha, DI21C-08, AGU, San Francisco, Dec. 14., 2010.
 27. Beyond Band Theory for Minerals at High Pressures, AGU, San Francisco, Dec. 16, 2010.
 28. First-principles theory, statistical mechanical modelling and experiments for design of new devices exploiting coupled phase transitions, Novel Electronic Devices Based on Coupled Phase Transitions Workshop, ONR, Jan.5-6, 2011.
 29. Metallization of FeO at high temperatures and pressures: DFT-DMFT computations and comparisons with experiments, Spring ACS Meeting, San Diego, March 27, 2012
 30. Metallization of FeO at high pressures and temperatures, Workshop on Novel Materials, UC Davis, June 24, 2012.
 31. Ferroelectricity under applied pressure and applied electric fields, 2012 International Workshop on Acoustic Transduction Materials and Devices, May 8, 2012.
 32. The electrocaloric effect under applied electric field and pressure, Drexel University, Department of Materials Science and Engineering, October 17, 2012.
 33. Effects of Mn on electromechanical properties of relaxor ferroelectrics, 2013 International Workshop On Acoustic Transduction Materials And Devices May 7, 2013, Penn State Univ.
 34. Properties of Iron under Core Conditions, Workshop on Elastic Properties of Iron in Extreme Conditions, 25 and 26 February, 2014, Takarazuka, Japan.
 35. Effects of Mn on Electromechanical Properties of Ferroelectrics, 31th Meeting on Ferroelectric Materials and Their Applications (FMA) (<http://fma.ceram.titech.ac.jp/>) 28 to 31 May, 2014, Kyoto, Japan.
 36. Behaviour of transition metals and transition metal oxides under pressure, and effects on transition metal dopants on ferroelectrics, Waseda University, May, 2014.
 37. Importance of electron correlations in iron compounds: DFT/DMFT computations, CSEC, University of Edinburgh, May 14, 2014.
 38. Behaviour of transition metals and transition metal oxides under pressure, University of Tokyo, Japan, May 23, 2014.
 39. Is PPv the last mantle phase transition? PPv@10: A meeting for the 10th anniversary of the discovery of post-perovskite, University of Bristol, June 26, 2014.
 40. Quantum Monte Carlo simulations on silicate perovskite and other high pressure phases, Quantum Monte Carlo in the Apuan Alps IX, July 30, 2014, TTI, Vallico Sotto, Tuscany, Italy
 41. Quantum Monte Carlo for Materials at High Pressures, Dept. Physics, Rutgers University, Nov 18, 2014.

42. Effects of electron correlations on iron and iron-bearing minerals in the Earth, Earth Science Institute, Hebrew University, Jerusalem, Israel, March 16, 2015.
43. Theory of large coupling ferroelectrics, Dept. of Applied Physics, Hebrew University, Jerusalem, Israel, March 19, 2015.
44. Equation of state and phase transitions of (Mg,Fe)SiO₃ perovskite and post-perovskites from quantum Monte Carlo and Density Functional Theory, 2015 Joint Assembly Meeting, AGU, 2015.
45. Pressure on Correlated Materials: Transport in iron and implications for the geodynamo, and electronic transitions in iron compounds, Keynote speaker, Joint AIRAPT-25-EHPRG-53, Madrid, Spain, 2015.
46. Quantum Monte Carlo for Materials at High Pressures, Cohen, Psi-k Conference, Sept. 6-10, 2015, Donostia-San Sebastián, Spain.
47. Electrical conductivity in the mantle and core and implications for the geodynamo, AGU Fall Meeting, San Francisco, Invited, 2015.
48. Equations of state and phase transitions in (Mg,Fe)SiO₃ perovskite and post-perovskites, position of the phase boundary and its double crossing, by Quantum Monte Carlo, AGU Fall Meeting, San Francisco, Invited, 2015.
49. Electrical conductivity in the mantle and core and implications for the geodynamo, "The Earth's Mantle and Core: Structure, Composition, Evolution" Matsuyama, Japan, November 4-7, 2015.
50. Electrical conductivity in the mantle and core and implications for the geodynamo, Outer Core Observations, Structure, Composition, 15th Symposium of SEDI, Nantes, France, on July 24 – 29, 2016.

Prizes and Fellowships Last 10 years

International Award of Ferroelectric Materials and Their Applications, FMA, May 29, 2014
 Dana Medal, Mineralogical Society of America, 2009