Curriculum Vitae

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Born: April 1, 1961

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Employment

December 2013-present	Rutgers University, Board of Governors Professor of Physics
January 2000-December 2013	Rutgers University, Professor of Physics
July 1999-January 2000	Yale University, Professor of Applied Physics and Physics
July 1995-July 1999	Yale University, Associate Professor of Applied Physics and Physics (tenured)
July 1993-July 1995	Yale University, Clare Boothe Luce Associate Professor of Applied Physics and Physics (term)
Sept. 1989-July 1993	Yale University, Clare Boothe Luce Assistant Professor of Applied Physics and Physics
Sept. 1987-Sept. 1989	AT&T Bell Laboratories, Postdoctoral Member of Technical Staff, Theoretical Physics Department

Education

Sept. 1982-Sept. 1987	PhD. in Physics, Massachusetts Institute of Technology "Ab initio Statistical Mechanics of Structural Phase Transitions" Thesis supervisor: John D. Joannopoulos
Sept. 1978-June 1982	A.B. in Physics, magna cum laude, Princeton University

Academic Honors

National Academy of Sciences, member	2013
American Academy of Arts and Sciences, member	2013
Fellow of the AAAS	2011
David Adler Lectureship Award in Materials Physics	2008
Promotion from Professor I to Professor II, Rutgers University	2004
Fellow of the American Physical Society	2003
Arthur Greer Memorial Prize, Yale College	1994
Alfred P. Sloan Research Fellowship	1993
Junior Faculty Fellowship in the Natural Sciences, Yale Univ.	1991
Presidential Young Investigator	1990
Clare Boothe Luce Professorship (five-year term)	1989
Phi Beta Kappa	1982
George B. Wood Legacy Prize (first in junior class)	1982
N.S.F. Graduate Fellowship	1982
Ida M. Green Fellowship	1982
AT&T Graduate Research Program for Women, fellowship	1982

Publications

1. "Ab initio relativistic pseudopotential study of the zero-temperature structural properties of SnTe and PbTe," K. M. Rabe and J. D. Joannopoulos, *Phys. Rev. B* 32, 2302 (1985).

2. "Ab initio statistical mechanics of GeTe," K. M. Rabe, J. D. Joannopoulos and A. Nihat Berker, *Proceedings of the 18th International Conference on the Physics of Semiconductors, Stockholm, Sweden* (World Scientific, 1987), p. 1221.

3. "Structural properties of GeTe at T=0," K. M. Rabe and J. D. Joannopoulos, *Phys. Rev. B* 36, 3319 (1987).

4. "Ab initio determination of a structural phase transition temperature," K. M. Rabe and J. D. Joannopoulos, *Phys. Rev. Lett.* 59, 570 (1987).

5. "Theory of the structural phase transition of GeTe," K. M. Rabe and J. D. Joannopoulos, *Phys. Rev. B* 36, 6631 (1987).

6. "Ab initio statistical mechanics of structural phase transitions," K. M. Rabe and J. D. Joannopoulos, *Electronic Phase Transitions,* ed. by W. Hanke and Y. V. Kopaev, (North-Holland, Amsterdam, 1992), Chap. 3.

7. "Superconductivity and lattice distortions in high-T_c superconductors," A. J. Millis and K. M. Rabe, *Phys. Rev. B* 38, 8908 (1988).

8. "Structural anomalies at the disappearance of superconductivity in $Ba_2YCu_3O_{7-d}$: evidence for charge transfer from chains to planes," R. J. Cava, B. Batlogg, K. M. Rabe, E. A. Rietman, P. K. Gallagher and L. W. Rupp, Jr., *Physica C* 156, 523 (1988).

9. "Studies of oxygen-deficient $Ba_2YCu_3O_{7-d}$ and superconductivity in Bi(Pb)-Sr-Ca-Cu-O," R. J. Cava, B. Batlogg, S. A. Sunshine, T. Siegrist, R. M. Fleming, K. Rabe, et al., *Physica C* 153-155, 560 (1988).

10. "Optimized pseudopotentials," A. M. Rappe, K. M. Rabe, E. Kaxiras and J. D. Joannopoulos, *Phys. Rev. B* 41, 1227 (1990).

11. "Structural anomalies, oxygen ordering and superconductivity in oxygen-deficient $Ba_2YCu_3O_{7-d}$", R. J. Cava, A. W. Hewat, E. A. Hewat, B. Batlogg, M. Marezio, K. M. Rabe, J. J. Krajewski, W. F. Peck, Jr., L. W. Rupp, Jr., *Physica C* 165, 419 (1990).

12. "Quantum diagrams and the prediction of new ternary quasicrystals," K. M. Rabe, A. R. Kortan, J. C. Phillips and P. Villars, *Phys. Rev. B* 43, 6280 (1991).

13. "Impurity states and magnetic order in layered copper oxides," K. M. Rabe and R. N. Bhatt, *J. App. Phys*. 69, 4508 (1991).

14. "Transport anomalies and structural models of stable quasicrystals," J. C. Phillips and K. M. Rabe, *Phys. Rev. Lett.* 66, 923 (1991).

15. "Anomalous properties and microstructural model of superconductivity in $La_{2-x}(Ba,Sr)_x Cu O_4$," J. C. Phillips and K. M. Rabe, *Phys. Rev. B* 44, 2863 (1991).

16. "Chemical trends in high-T_c ferroelectricity and superconductivity," P. Villars, J. C. Phillips, K. M. Rabe and I.D. Brown, *Ferroelectrics* 130, 129 (1992).

17. "Global multinary structural chemistry of stable quasicrystals, high-T_c ferroelectrics and superconductors," K. M. Rabe, J. C. Phillips, P. Villars and I. D. Brown, *Phys. Rev. B* 45, 7650 (1992).

18. "Structures and phases of superconducting alkali - metal doped C_{60}," K. M. Rabe, J. C. Phillips and J. M. Vandenberg, *Phys. Rev. B* 47, 13067 (1993).

19. "First-principles model Hamiltonians for ferroelectric phase transitions," K. M. Rabe and U. V. Waghmare, *Ferroelectrics* 136, 147 (1992).

20. "Quantum diagrams, structural models and the prediction of new quasicrystals," K. M. Rabe, J. C. Phillips and P. Villars, *Journal of Noncrystalline Solids* 153 & 154, 530 (1993).

21. "Quantum diagrams and the prediction of new materials," K. M. Rabe, *Journal of Alloys and Compounds* 197, 131 (1993).

22. "Novel A15 phase in barium-doped fullerite," A. R. Kortan, N. Kopylov, R. M. Fleming, O. Zhou, F. A. Thiel, R. C. Haddon, and K. M. Rabe, *Phys. Rev. B* 47, 13070 (1993).

23. "Theory and practice in the prediction of new materials," K. M. Rabe, *MRS Bulletin,* February 1993, p. 31 (cover story).

24. "First-principles model Hamiltonians for ferroelectric transitions," K. M. Rabe and U. V. Waghmare, *Ferroelectrics* 151, 69 (1994).

25. "Ferroelectric phase transitions: a first-principles approach," K. M. Rabe and U. V. Waghmare, *Ferroelectrics*, 164, 15 (1995).

26. "Coulomb interaction and ferroelectric phase transitions in perovskite compounds," W. Zhong, D. Vanderbilt, R. D. King-Smith, and K. M. Rabe, *Ferroelectrics*, 164, 291 (1995).

27. "Ab initio pseudopotential calculations for aluminium-rich cobalt compounds," S. Ogut and K. M. Rabe, *Phys. Rev. B* 50, 2075 (1994).

28. "Phase transitions in $BaTiO_3$ from first principles," W. Zhong, D. Vanderbilt and K. M. Rabe, *Phys. Rev. Lett.* 73, 1861 (1994).

29. "First principles study of structural energetics and transport properties of intermetallic compounds," S. Ogut and K. M. Rabe, *Turk. J. Phys.* 19, 74 (1995).

30. "Molecular orientational order in $K_4 C_{60}$," K. M. Rabe, preprint.

31. "Band gap and stability in the ternary intermetallic compounds NiSnM (M = Ti, Zr, Hf): A first principles study," S. Ogut and K. M. Rabe, *Phys. Rev B* 51, 10443 (1995).

32. "Localized basis for effective lattice Hamiltonians: lattice Wannier functions," K. M. Rabe and U. V. Waghmare, *Phys. Rev B* 52, 13236 (1995).

33. "First principles theory of ferroelectric phase transitions in perovskite compounds: The case of $BaTiO_3$" W. Zhong, D. Vanderbilt and K. M. Rabe, *Phys. Rev B* 52, 6301 (1995).

34. "Optical properties of quasicrystalline semiconductors," K. M. Rabe, S. Ogut and J. C. Phillips, in *Prcceedings of the 5th International Conference on Quasicrystals,* ed. by C. Janot and R. Mosseri, World Scientific, Singapore, 1995, p. 613.

35. "Polymorphism and metastability in NbN: structural predictions from first principles," S. Ogut and K. M. Rabe, *Phys. Rev B* 52, R8585 (1995).

36. "Superconductivity and cation-vacancy ordering in the rare earth fulleride $Yb_{2.75}C_{60}$," E. Ozdas, A. R. Kortan, N. Kopylov, A. P. Ramirez, T. Siegrist, K. M. Rabe, H. E. Bair, S. Schuppler and P. H. Citrin, *Nature* 375, 126 (1995).

37. "Ferroelectric phase transitions from first principles," K. M. Rabe and U. V. Waghmare, J. Phys. Chem. Solids 57, 1397 (1997).

38. "Strain coupling in the $PbTiO_3$ ferroelectric transition," K. M. Rabe and U. V. Waghmare, Phil. Trans. Roy. Soc. Lond. A354, 2897 (1996).

39. "Lattice instabilities, anharmonicity and phase transitions in $PbZrO_3$ from first principles," U. V. Waghmare and K. M. Rabe, Ferroelectrics 194, 135 (1997).

40. "Strain coupling in perovskite structural transitions: a first-principles approach," K. M. Rabe and U. V. Waghmare, Ferroelectrics 194, 119 (1997).

41. "Anomalous effective charges and far IR optical absorption of Al_2Ru from first principles," S. Ogut and K. M. Rabe, Phys. Rev. B54, R8297 (1996).

42. "Ab initio statistical mechanics of the ferroelectric phase transition in $PbTiO_3$," U. V. Waghmare and K. M. Rabe, Phys. Rev. B55, 6161 (1997).

43. "Ab initio study of the structural phase transition in cubic Pb_3GeTe_4," E. Cockayne and K.M. Rabe, Phys. Rev. B56, 7947 (1997).

44. "Vacancy-induced structural relaxations in $Yb_{2.75}C_{60}$," K.M. Rabe and P.H. Citrin, Phys. Rev. B--Rapid Communications 58, R551 (1998).

45. "Enhancement of piezoelectricity in a mixed ferroelectric," E. Cockayne and K. M. Rabe, Phys. Rev. B--Rapid Communications 57, R13973 (1998).

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51. "First-principles investigation of ferromagnetism and ferroelectricity in bismuth manganite," N. A. Hill and K. M. Rabe, Phys. Rev. B59, 8759 (1999).

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53. "Lattice dynamics of $BaTiO_3$, $PbTiO_3$, and $PbZrO_3$: a comparative first-principles study," Ph. Ghosez, E. Cockayne, U. V. Waghmare and K. M. Rabe, Phys. Rev. B60, 836 (1999).

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122. June Hyuk Lee, L. Fang, E. Vlahos, X. L. Ke, Y. W. Jung, L. F. Kourkoutis, J. W. Kim, P. J. Ryan, T. Heeg, M. Roeckerath, V. Goian, M. Bernhagen, R. Uecker, P. C. Hammel, K. M. Rabe, S. Kamba, J. Schubert, J. W. Freeland, D. A. Muller, C. J. Fennie, P. Schiffer, V. Gopalan, E. Johnston-Halperin and D. G. Schlom, "A strong ferroelectric ferromagnet created by means of spin-lattice coupling," Nature 466, 954 (2010).

123. L. Pálová, P. Chandra and K. M. Rabe, "Multiferroic $BiFeO_3$-$BiMnO_3$ nanoscale checkerboard from first principles," Phys. Rev. B 82, 075432 (2010). (Editor's Suggestion)

124. X. F. Wu, K. M. Rabe and D. Vanderbilt, "Interfacial enhancement of ferroelectricity in $CaTiO_3$/$BaTiO_3$ superlattices," Phys. Rev. B 83, 020104 (2011).

125. Jun Hee Lee and K. M. Rabe, "Coupled magnetic-ferroelectric metal-insulator transition in epitaxially-strained $SrCoO_3$ from first principles," Phys. Rev. Lett. 107, 067601 (2011).

126. Jun Hee Lee and K. M. Rabe, "Large spin-phonon coupling and magnetically-induced phonon anisotropy in $SrMO_3$ perovskites (M=V, Cr, Mn, Fe, Co)," Phys. Rev. B 84, 104440 (2011). (Editor's Suggestion)

127. Jeroen L. Blok, Karin M. Rabe, David Vanderbilt, Dave H. A. Blank and Guus Rijnders, ``Interplay of epitaxial strain and rotations in $PbTiO_3$/$PbZrO_3$ superlattices from first principles," Phys. Rev. B 84, 205413 (2011).

128. A. Kumar, C. J. Fennie, and K. M. Rabe, "Spin-lattice coupling and phonon dispersion of $CdCr_2O_4$ from first principles," Phys. Rev. B 86, 184429 (2012)

129. Yijia Gu, Karin Rabe, Eric Bousquet, Venkatraman Gopalan, and Long-Qing Chen, "Phenomenological thermodynamic potential for $CaTiO_3$ single crystals," Phys. Rev. B 85, 064117 (2012).

130. A. Ignatov, A. Kumar, P. Lubik, R. H. Yuan, W. T. Guo, N. L. Wang, K. Rabe, and G. Blumberg, "Structural phase transition below 250 K in superconducting $K_{0.75}Fe_{1.75}Se_2$," Phys. Rev. B 86, 134107 (2012).

131. Joseph W. Bennett and Karin M. Rabe, "Integration of first-principles methods and crystallographic database searches for new ferroelectrics: Strategies and explorations," J. Solid State Chem. 195, 21 (2012).

132. Anindya Roy, Joseph W. Bennett, Karin M. Rabe and David Vanderbilt, "Half-Heusler semiconductors as piezoelectrics," Phys. Rev. Lett. 109, 037602 (2012).

133. Joseph W. Bennett, Kevin F. Garrity, Karin M. Rabe, David Vanderbilt, "Hexagonal ABC compounds as ferroelectrics," Phys. Rev. Lett. 109, 167602 (2012). (Editor's Suggestion and Physics Synopsis)

134. K. M. Rabe, "Antiferroelectricity in oxides: A reexamination," in *Functional Metal Oxides: New Science and Applications*, eds. S. Ogale and V. Venkateshan (Wiley, 2013).

135. Joseph W. Bennett, Kevin F. Garrity, Karin M. Rabe, David Vanderbilt, "Orthorhombic ABC semiconductors as antiferroelectrics," Phys. Rev. Lett. **110**, 017603 (2013).

136. Anil Kumar, Karin M. Rabe, and Umesh V. Waghmare, "Domain formation and dielectric response in $PbTiO_3$: A first-principles free-energy landscape analysis," Phys. Rev. B 87, 024107 (2013). (Editor's Suggestion)

137. Woo Seok Choi, Hyoungjeen Jeen, Jun Hee Lee, S. S. Ambrose Seo, Valentino R. Cooper, Karin M. Rabe, and Ho Nyung Lee, "Reversal of the lattice structure in $SrCoO_x$ epitaxial thin films studied by real-time optical spectroscopy and first-principles calculations," Phys. Rev. Lett. 111, 097401 (2013).

138. Yuanjun Zhou and Karin M. Rabe, "Epitaxial strain effects on magnetic ordering and spin-phonon couplings in the $(LaMnO_3)_1(SrMnO_3)_1$ superlattice from first principles," Phys. Rev. B 88, 094416 (2013).

139. Sebastian E. Reyes-Lillo and Karin M. Rabe, "Antiferroelectricity and ferroelectricity in epitaxially strained $PbZrO_3$ from first principles," Phys. Rev. B 88, 180102(R) (2013).

140. Jun Hee Lee, Kris T. Delaney, Eric Bousquet, Nicola A. Spaldin, and Karin M. Rabe, Strong coupling of Jahn-Teller distortion to oxygen-octahedron rotation and functional properties in epitaxially strained orthorhombic $LaMnO_3$, Phys. Rev. B 88, 174426 (2013).

141. S. Kamba, V. Goian, V. Skoromets, J. Hejtmánek, V. Bovtun, M. Kempa, F. Borodavka, P. Vaněk, A. A. Belik, J. H. Lee, O. Pacherová, and K. M. Rabe, "Strong spin-phonon coupling in infrared and Raman spectra of $SrMnO_3$," Phys. Rev. B 89, 064308 (2014).

142. K. F. Garrity, K. M. Rabe and D. Vanderbilt, "Hyperferroelectrics: Proper ferroelectrics with persistent polarization," Phys. Rev. Lett. 112, 127601 (2014). (Editor's Suggestion, Featured in Physics)

143. Sebastian E. Reyes-Lillo, Kevin F. Garrity, and Karin M. Rabe, "Antiferroelectricity in thin-film ZrO_2 from first principles," Phys. Rev. B 90, 140103 (2014). (Rapid Communication, Editor's Suggestion)

144. Kevin F. Garrity, Joseph W. Bennett, Karin M. Rabe and David Vanderbilt, "Pseudopotentials for high-throughput DFT calculations," Comp. Mat. Sci. 81, 446 (2014).

145. H. Shimizu, H. Z. Guo, S. E. Reyes-Lillo, Y. Mizuno, K. M. Rabe and C. A. Randall, "Lead-free antiferroelectric: $xCaZrO_3$-$(1-x)NaNbO_3$ system ($0<=x<=0.10$)," Dalton Transactions 44, 10763 (2015).

146. Yuanjun Zhou and Karin M. Rabe, "Determination of ground-state and low-energy structures of perovskite superlattices from first principles," Phys. Rev. B 89, 104108 (2014).

147. Yuanjun Zhou, Karin M. Rabe and David Vanderbilt, "Surface polarization and edge charges," Phys. Rev. B 92, 041102 (2015).

148. Yuanjun Zhou and Karin M. Rabe, "Coupled nonpolar-polar metal-insulator transition in 1:1 $SrCrO_3/SrTiO_3$ superlattices: A first-principles study," Phys. Rev. Lett. 115, 106401 (2015).

149. S. Ismail-Beigi, F. J. Walker, S. W. Cheong, K. M. Rabe and C. H. Ahn, "Alkaline earth stannates: The next silicon?" APL Materials 3, 062510 (2015).

150. L. Zhang, Y. J. Zhou, L. Guo, W. W. Zhao, A. Barnes, H. T. Zhang, C. Eaton, Y. X. Zheng, M. Brahlek, H. F. Haneef, N. J. Podraza, M. H. W. Chan, V. Gopalan, K. M. Rabe and R. Engel-Herbert, "Correlated metals as transparent oxides," Nature Materials 15, 204 (2016).

151. H. Wang, J. Wen, D. J. Miller, Q. Zhou, M. Chen, H. N. Lee, K. M. Rabe and X. Wu, "Stabilization of highly polar $BiFeO_3$-like structure: a new interface design route for enhanced ferroelectricity in artificial perovskite superlattices, Phys. Rev. X, in press.

Books

"Physics of Ferroelectrics: a Modern Perspective," editors K. M. Rabe, C. H. Ahn and J. M. Triscone, Topics in Applied Physics 105 (Springer Verlag 2007).
Coauthor of two chapters:
"Modern physics of ferroelectrics: essential background," with M. Dawber, C. Lichtensteiger, C. H. Ahn and J. M. Triscone (pp. 1-30).
"First principles studies of ferroelectric oxides," with Ph. Ghosez (pp. 117-174)

Invited Talks

1. K. M. Rabe, "Ab initio statistical mechanics of GeTe," American Physical Society meeting, New Orleans, Louisiana, March 1988.

2. J. D. Joannopoulos and K. M. Rabe, "Ab initio statistical mechanics," Materials Research Society Meeting, Boston, Massachusetts, December 1988.

3. K.M. Rabe and R.N. Bhatt, "Impurity states and magnetic order in layered copper oxides," Conference on Magnetism and Magnetic Materials, San Diego, California, October 1990.

4. K.M. Rabe, "Quantum diagrams and the prediction of new quasicrystals, ferroelectrics and superconductors," Minerals, Metals and Materials Society Annual Meeting, San Diego, California, March 1992.

5. K.M. Rabe, "Internal structural models of superconductive cluster compounds," American Physical Society meeting, Indianapolis, Indiana, March 1992.

6. K.M. Rabe, "Quantum diagrams and the prediction of new quasicrystals, ferroelectrics and superconductors", Workshop on Regularities, Classifications and Predictions of Advanced Materials, Como, Italy, April 1992.

7. K.M. Rabe, "Quantum diagrams and the prediction of new quasicrystals," 4th International Conference on Quasicrystals, St. Louis, Missouri, June 1992.

8. K.M. Rabe, "First-principles calculation of ferroelectric transitions," 8th International Meeting on Ferroelectricity, Gaithersburg, Maryland, August 1993.

9. K. M. Rabe, "Ferroelectric phase transitions: a first-principles approach," Third Williamsburg Workshop on First-principles Calculations for Ferroelectricity, Williamsburg, Virginia, February 1994.

10. K.M. Rabe, "Quantum diagrams and the prediction of new materials," Second MOE Workshop, Kyoto, Japan, March 1994.

11. K. M. Rabe, "Ferroelectric phase transitions: a first-principles approach," International Symposium on Integrated Ferroelectrics, Monterey, California, March 1994.

12. K. M. Rabe, "Ferroelectric phase transitions: a first-principles approach," American Ceramic Society meeting, Indianapolis, Indiana, 1994.

13. K. M. Rabe, "Quantum diagrams and the prediction of new materials," 1994 American Crystallographic Association meeting, Atlanta, Georgia, June 1994.

14. S. Ogut and K. M. Rabe, "First principles study of structural energetics and transport properties of intermetallic compounds," Second Turkish Conference on Statistical Physics, Istanbul, Turkey, July 1994.

15. D. Vanderbilt, W. Zhong and K. M. Rabe, "Structural phase transitions in ferroelectric perovskites," Materials Research Society, Fall Meeting, Boston, Massachusetts, December 1994.

16. K. M. Rabe, "Lattice Wannier functions and the ferroelectric transition in $PbTiO_3$," Seventh International Workshop on Computational Condensed Matter Physics Based on the Electronic Structure, ICTP, Trieste, Italy, January 1995.

17. K. M. Rabe, "Ferroelectric phase transitions from first principles," Workshop on Fundamental Experiments on Ferroelectrics, Williamsburg, Virginia, February 1995.

18. K. M. Rabe, "Diagrammatic approaches to the prediction of new materials," Hume-Rothery Award Symposium for Professor David Pettifor, Minerals, Metals and Materials Society Annual Meeting, Las Vegas, Nevada, February 1995.

19. K. M. Rabe, "Ferroelectric phase transitions from first principles," Mardi Gras Conference on High Performance Computing Technologies and Scientific Applications, Baton Rouge, Louisiana, February 1995.

20. K. M. Rabe, "Ferroelectric phase transitions from first principles," IV International Conference on Advanced Materials (ICAM-4), Cancun, Mexico, August 1995.

21. K. M. Rabe, "Lattice instabilities, anharmonicity and phase transitions in $PbTiO_3$ and $PbZrO_3$: an ab initio statistical mechanics study," Materials Research Society, Fall Meeting, Boston, Massachusetts, December 1995.

22. U. V. Waghmare and K. M. Rabe, "Lattice instabilities, anharmonicity and phase transitions in $PbZrO_3$ from first principles,", Fourth Williamsburg Workshop on First-Principles Calculations for Ferroelectricity, Williamsburg, Virginia, February 1996.

23. K. M. Rabe, "Strain coupling in perovskite structural transitions: a first-principles approach," Fourth Williamsburg Workshop on First-Principles Calculations for Ferroelectricity, Williamsburg, Virginia, February 1996.

24. K. M. Rabe, "Lattice instabilities, anharmonicity and phase transitions in $PbTiO_3$, $PbZrO_3$ and $Pb_{1-x}Ge_xTe$," CECAM Workshop on Ab Initio Phonons, Lyon, France, July 1996.

25. K. M. Rabe, "Water clusters," Workshop on Recent Developments in Pseudopotential Theory, Rockport, Massachusetts, October 1996.

26. K. M. Rabe, ``Ferroelectric phase transitions from first principles, "Applied Mathematics Workshop for Materials Studies and Industrial Applications, Pennsylvania State University, October 1996.

27. K. M. Rabe and E. Cockayne, ``Ferroelectricity and piezoelectricity in substitutionally disordered $Pb_{0.75}Ge_{0.25}Te$," Third Williamsburg Workshop on Fundamental Experiments in Ferroelectricity, Williamsburg, Virginia, February 1997.

28. K. M. Rabe, ``Ferroelectric phase transitions from first principles," American Physical Society March Meeting, Kansas City, Missouri, March 1997.

29. K. M. Rabe, ``Ferroelectric phase transitions from first principles," Ninth Annual Workshop on Recent Developments in Electronic Structure Algorithms, Ithaca, New York, May 1997.

30. K. M. Rabe, "First-principles effective Hamiltonians for ferroelectrics and piezoelectrics," CECAM Workshop on First-Principles Theory of Ferroelectric Materials, Lyon, France, July 1997.

31. K. M. Rabe and E. Cockayne, ``Temperature-dependent piezoelectric and dielectric response of ferroelectrics from first principles," Fifth Williamsburg Workshop on First-Principles Calculations for Ferroelectricity, Williamsburg, Virginia, February 1998.

32. K. M. Rabe, ``Temperature-dependent piezoelectric and dielectric response of ferroelectrics from first principles," 1998 ONR Transducer Materials and Transducers Workshop, Pennsylvania State University, May 1998.

33. K. M. Rabe, `` Ferroelectricity in $PbTiO_3$ thin films: a first-principles approach," 5^{th} International Workshop on Oxide Electronics, College Park, Maryland, December 1998.

34. K. M. Rabe and Ph. Ghosez, ``Interatomic force constants and microscopic models of ferroelectricity in perovskite thin films and solid solutions," Materials Research Society Fall Meeting, Boston, Massachusetts, December 1999.

35. K. M. Rabe and Ph. Ghosez, ``Ferroelectricity in ultrathin $PbTiO_3$ films: a first principles approach," Aspen Center for Physics Winter Conference on Fundamental Physics of Ferroelectrics, Aspen, Colorado, February 2000.

36. K. M. Rabe and Ph. Ghosez, ``Microscopic effective Hamiltonians for ferroelectrics from first principles," Materials Research Society Spring Meeting, San Francisco, California, April 2000.

37. K. M. Rabe and Ph. Ghosez, ``A microscopic model of ferroelectricity in $PbTiO_3$ thin films," Materials Research Society Spring Meeting, San Francisco, California, April 2000.

38. K. M. Rabe, ``Microscopic models for ferroelectrics from first principles," Workshop on Computational Materials: Fundamentals, Evolution and Design, Princeton Materials Institute, Princeton, New Jersey, May 2000.

39. K. M. Rabe and V. Godlevsky, ``First-principles effective Hamiltonians for magnetic martensites," 3rd SIAM Conference on Materials Science, Philadelphia, Pennsylvania, May 2000.

40. K. M. Rabe and U. V. Waghmare, ``Lattice Wannier functions: a method for constructing effective lattice Hamiltonians from first principles," NIST Effective Hamiltonian Workshop, Gaithersburg, Maryland, May 2000.

41. K. M. Rabe and C. Bungaro, "Improving first-principles effective Hamiltonians: Lattice dynamics of PZT," Williamsburg 2001 Workshop on Fundamental Physics of Ferroelectrics, Williamsburg, VA, February 2001.

42. K. M. Rabe, C. Bungaro and J. Neaton, "Ferroelectricity & piezoelectricity in ultrathin films and superlattices from first principles, MRS Workshop on Dielectric Science and New Functionality in Device Physics for Crystalline Oxides on Semiconductors, Chattanooga, Tennessee, September 2001.

43. K. M. Rabe, C. Bungaro and J. Neaton, "Polarization and dielectric response of atomic-scale perovskite heterostructures by design," Fundamental Physics of Ferroelectrics 2002, Washington, DC, February 2002.

44. K. M. Rabe, C. Bungaro and J. Neaton, "Perovskite ultrathin films and superlattices from first principles," Materials Research Society Spring 2002 meeting, San Francisco, CA, April 2002.

45. K. M. Rabe, C. Bungaro and J. Neaton, "Perovskite ultrathin films and superlattices from first principles," DARPA/ONR Workshop on First Principles Design of Materials, Arlington, VA, May 2002.

46. K. M. Rabe, "Polarization and dielectric response of perovskite oxide superlattices "by design"," 9th International Workshop on Oxide Electronics, St. Petersburg, Florida, October 2002.

48. K. M. Rabe, "Statistical mechanics of real materials," 89th Statistical Mechanics Meeting, Rutgers University, November 2002.

49. K. M. Rabe, "Lattice instabilities of complex oxides from first principles," 16th Annual Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics, U. Georgia, February 2003.

50. K. M. Rabe, "Structure and function from first principles," Workshop on Nonequilibrium Interface Dynamics: Theory and Simulation from Atomistic to Continuum Scales, Center for Scientific Computation and Mathematical Modeling, University of Maryland, October 2003.

51. K. M. Rabe, "Structural phase transitions in epitaxial perovskite thin films and superlattices from first principles,' ONR Workshop on Frontiers of Epitaxial Engineering, Moab, Utah, May 2004.

52. K. M. Rabe, "Microscopic and macroscopic first-principles modeling of functional oxide thin films and superlattices," MRS Fall Meeting, Boston, Massachusetts, December 2004.

53. K. M. Rabe, "First-principles investigations of oxide thin films and superlattices and oxide multiferroics," DOE Workshop on Ferroelectricity at Small Length Scales, Santa Fe, New Mexico, June 2005.

54. K. M. Rabe, C.-J. Eklund, S. Li and C. J. Fennie, "Revealing hidden ferroelectricity in complex oxides,", Materials Research Society Fall Meeting, Boston, MA, November 2007.

55. K. M. Rabe, "Competing lattice instabilities and structural transitions in complex oxides from first principles," Williamsburg Workshop on Fundamental Physics of Ferroelectrics, Williamsburg, VA, February 2008.

56. K. M. Rabe, "Lattice instabilities and ferroelectricity in complex oxides," American Physical Society March Meeting, New Orleans, LA, March 2008.

57. K. M. Rabe, "Ferroelectric superlattices from first principles," 2008 SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, PA, May 2008.

58. K. M. Rabe, "Magnetostructural coupling in multiferroics, parts 1 and 2," ICMR Summer School on Multiferroics and Beyond, UCSB, July 20-August 1, 2008.

59. K. M. Rabe, C. J. Eklund, L. Palova and C. J. Fennie, "Novel functional oxide materials from first principles," Fall 2008 MRS Meeting, Boston, Massachusetts, November 2008.

60. K. M. Rabe, "Ferroelectricity and complex oxide surfaces and interfaces," Workshop on Functional Oxides for Renewable Energy Sciences and Technologies, Harvard University, March 5-6, 2009.

61. K. M. Rabe, Epitaxial-strain-induced ferroelectricity in complex oxides from first principles," Workshop on Atomistic Interfaces, University of Connecticut, August 2009.

62. K. M. Rabe, "Novel phase boundaries and functional properties in complex oxides from first principles," MRS Spring Meeting, San Francisco, California, April 2010.

63. K. M. Rabe, "Spin-lattice coupling in perovskite oxides from first principles," 103rd Statistical Mechanics Conference, Rutgers University, May 2010.

64. K. M. Rabe, "First principles theory and modeling of functional oxide materials," 2nd OxIDes Meeting, University of Geneva, Switzerland, May 2010.

65. K. M. Rabe, "Spin-lattice coupling in perovskite oxides from first principles," CECAM Workshop on Theory of Magnetoelectrics: Fundamentals and Applications, Lausanne, Switzerland, May 2010.

66. K. M. Rabe, "Materials with built-in competition: coupled phase transitions and functional properties," NSF-sponsored workshop on Materials by Design, University of California, Santa Barbara, March 2011.

67. K. M. Rabe, J. H. Lee, C.-J. Eklund and L. Palova, "Novel phase boundaries and functional properties in perovskite oxide superlattices from first principles," Materials Research Society Spring Meeting, San Francisco, California, April 2011.

68. Karin M. Rabe, "First-principles design of functional materials based on coupled first-order phase transitions," Materials Research Society Fall Meeting, Boston, Massachusetts, December 2011.

69. Karin M. Rabe, "Discovery and design of inorganic functional materials," Materials Genome Initiative Workshop on the Interplay of Experiment, Theory and Computation, National Science Foundation, Arlington, Virginia, December 2012.

70. Karin M. Rabe, "An antiferroelectric materials primer," Workshop on Fundamental Physics of Ferroelectrics and Related Materials, Ames, Iowa, January 2013

71. Karin M. Rabe, "New ferroelectrics and antiferroelectrics by design," 2013 NSF DMR MGI Workshop: The Materials Genome Initiative in Ceramics, Geosciences, and Solid-State Chemistry, Arlington, Virginia, February 2013.

72. Karin M. Rabe, "New ferroelectrics and antiferroelectrics by design," German Physical Society Meeting, Regensburg, Germany, March 2013.

73. Karin M. Rabe, “New ferroelectrics and antiferroelectrics by design,” Materials Research Society Spring Meeting, San Francisco, California, April 2013.

74. Karin M. Rabe, "New ferroelectrics and antiferroelectrics by design," AVS 60th International Symposium and Exhibition, Long Beach, CA, November 2013.

75. Karin M. Rabe, "New ferroelectrics and antiferroelectrics by design," 16th US-Japan Seminar on Dielectric and Piezoelectric Materials, North Carolina State University, Raleigh, NC November 2013

76. Karin M. Rabe, "Functional antiferroelectrics by design," KAST Korean-American Workshop, New York, NY, November 2013

77. Karin M. Rabe, "Functional antiferroelectrics by design," Materials Research Society Fall Meeting, Boston Massachusetts, December 2013.

78. Karin M. Rabe, "New ferroelectrics and antiferroelectrics by design," 110th Statistical Mechanics Conference, Rutgers University, Piscataway, NJ, December 2013.

79. Karin M. Rabe, "Age of Exploration: Materials discovery in the virtual world," Nanoday 2014, University of Maryland, College Park, MD, June 2014

80. Karin M. Rabe, “New functional materials from first principles,” Materials Science and Technology 2015, Columbus, Ohio, October 2015.

81. Karin M. Rabe, "Age of Exploration: Materials discovery in the virtual world," 2015 Annual Meeting of the APS Mid-Atlantic Section, Morgantown, West Virginia, October 2015 (plenary).

82. Karin M. Rabe, “Functional properties of superlattices from first-principles models,” Materials Research Society Fall Meeting, Boston, Massachusetts, November 2015.

83. Karin M. Rabe, “Functional superlattices from first principles,” Electronic Materials and Applications 2016, Orlando, Florida, January 2016.

Departmental Colloquia since 2010

1. K. M. Rabe, “Designer oxides that work,” Conference for Undergraduate Women in Physics, Massachusetts Institute of Technology, Cambridge, MA, January 15-16, 2011.
2. K. M. Rabe, “Phase transitions and functional behavior in complex oxides from first principles,” Summer Symposium on Chemistry and Physics of Functional Materials, University of California, Santa Barbara, July 26, 2011.
3. K. M. Rabe, “Discovery of new functional materials from first principles,” Department of Physics Colloquium, SUNY-Buffalo, October 25, 2012.

PhD Students Supervised

Serdar Ogut, PhD in Physics, Yale University, 1995. Upon graduation, obtained postdoctoral position at the University of Minnesota. Currently Professor of Physics at University of Illinois, Chicago Circle.

Umesh V. Waghmare, PhD in Applied Physics, Yale University, 1996. Upon graduation, obtained postdoctoral position at Harvard University. Currently Professor at J. Nehru Research Centre, Bangalore, India.

Craig J. Fennie, PhD program in Physics, Rutgers University, 2006. Currently Associate Professor of Engineering and Applied Sciences, Cornell University.

Carl-Johann Eklund, PhD program in Physics, Rutgers University, 2010.

Qibin Zhou, PhD program in Physics, Rutgers University, 2014. Currently Financial Software Engineer at Bloomberg L.P.

Yuanjun Zhou, PhD program in Physics, Rutgers University, 2015. Currently postdoctoral researcher at Columbia University.

Sebastian Reyes-Lillo, PhD program in Physics, Rutgers University, 2015. Currently postdoctoral researcher at Lawrence Berkeley Laboratory.

John Bonini, PhD program in Physics, Rutgers University, current.

Postdoctoral fellows supervised

Eric J. Cockayne 1995-1997; current position: Materials Scientist, NIST, Gaithersburg, MD.

Nicola Hill (now Spaldin) 1996; current position: Professor of Materials, ETH Zurich.

Philippe Ghosez 1998-1999; current position: Professor of Physics, Universite de Liege, Belgium

Vitaliy Godlevsky 1999-2001; current position: Quantitative Research Analyst, Quantlab Financial LLC, Houston, TX.

Jeffrey Neaton (co-supervised with D. Vanderbilt and D. Langreth) 2000-2003; current position: Lawrence Berkeley Laboratory and U. C. Berkeley.

Claudia Bungaro 2000-2004; current position: Web Developer at Atomic Software, NY

Xiangyang Huang 2001-2003; current position: Senior Physicist, RJ Mears LLC, Waltham, MA

Ivan I. Naumov 2001-2003; current position: Research Scientist, Carnegie Institution of Washington

Silvia Tinte (co-supervised with D. Vanderbilt) 2001-2004; current position: Universidad Nacional del Litoral, Argentina

Javier Junquera, 2003-2005, current position: Profesor Titular de Universidad, Universidad de Cantabria, Spain

Karen Johnston, 2003-2005, current position: Lecturer, University of Strathclyde, Glasgow, Scotland.

Alexey Zayak, 2004-2006, current position: Assistant Professor, Physics and Astronomy Department, Bowling Green State University

Serge Nakhmanson (co-supervised with D. Vanderbilt) 2004-2006, current position: Associate Professor, Department of Materials Science and Engineering, University of Connecticut

Timo Thonhauser (co-supervised with D. Vanderbilt and D. Langreth) 2004-2008, current position, Associate Professor of Physics, Wake Forest University

Shen Li (co-supervised with D. Langreth) 2005-2008, current position: University of Washington.

Valentino Cooper (co-supervised with D. Langreth) 2005-2008, current position: Staff Scientist, Oak Ridge National Laboratory.

Oscar Paz, 2008-2010, current position: Insitut de Ciencia de Materials de Barcelona.

Jun Hee Lee, 2008-2011, current position: Oak Ridge National Laboratory.

Joseph W. Bennett, 2010-2012 and 2015-present (staff scientist).

Anil Kumar, 2010-2013, current position: Postdoctoral Researcher, Los Alamos National Laboratory.

Yanpeng Yao, 2011-2013

Kevin Garrity, 2011-2014, current position: Research Assoicate, NIST, Gaithersburg, Maryland

Sergey Artyukhin, 2011-2015, current position: Researcher, Italian Institute of Technology, Genoa, Italy

Jialan Zhang, 2015-present

Se Young Park, 2015-present

Xiaohui Liu, 2016-present

Current grant support

ONR "Novel functional materials from first principles," 8/31/12 - 12/31/16, $645,277.

ONR "Polarization-switched conductivity at perovskite-oxide interfaces: Optimization through materials design," 7/01/14 - 12/31/16, $312,500.

ONR (subcontract from Yale), "Ferroelectric control of Mott transitions and magnetic order in correlated oxide based devices," 6/01/2011-5/30/16, $540,000

NSF (DMREF program), "High-throughput mapping of functional dielectric/metallic heterostructures," 9/1/13-8/31/17, $475,000 (co-PI P. Chandra)

Professional activities since 2005

Aspen Center for Physics: General Member (since 1995), Trustee (2002-2008), Vice President (2007-2013), President (2013-present).

Co-organizer (with E. Cockayne, P. Gehring, R. Cohen and Z. G. Ye), Workshop on the Fundamental Physics of Ferroelectrics, Washington, DC, January 2013.

Co-organizer (with J. Moore, C. Nayak, A. Cavalleri, and G. Aeppli), Winter Conference on New Paradigms in Low-Dimensional Electronic Materials, Aspen, CO, February 2012.

Co-organizer (with R. E. Cohen, P. Gehring and D. Schlom), Winter Conference on Advances in Fundamental Physics of Ferroelectrics and Beyond, Aspen, CO, January 2010.

Co-organizer (with P. Davies), 18th Annual Workshop on Fundamental Physics of Ferroelectrics, Williamsburg, VA, February 2007.

Co-organizer (with T. Shrout), 16th Annual Workshop on Fundamental Physics of Ferroelectrics, Williamsburg, VA, February 2005.

Editorial Board, Physical Review B, 2003-2009.

Journal of Physics: Condensed Matter, member of Advisory Editorial Board, 2003-2007.

Max Planck Institute for the Structure and Dynamics of Matter (Hamburg, Germany), Advisory Board member, 2016 – present

Army Research Laboratory, Advisory Board member, 2015 – present

Argonne National Laboratory: Physical Sciences and Engineering Directorate Review Committee member, 2011-present

EPSRC Portfolio Grant in Theoretical Physics and Chemistry at the University of Cambridge, visiting committee, 2004-2008.

CMMP 2010: An Assessment of and Outlook for Condensed-Matter and Materials Physics (National Academy of Science), committee member.

Oliver E. Buckley Condensed Matter Prize committee, American Physical Society: member 2010, chair 2011.

David Adler Lectureship Award committee, American Physical Society: member 2008.

Referee of articles for Nature, Science, Physical Review Letters, Applied Physics Letters, Physical Review B, Solid State Communications

Referee of grants for National Science Foundation, Department of Energy, US-Israel Binational Science Foundation, EPSRC

K-12 Outreach
Co-coach of Science Bowl team, Highland Park Middle School, Fall 2012 to the present