

Curriculum Vitae

Name: Karin M. Rabe

Address: Rutgers University
Department of Physics and Astronomy
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Born: April 1, 1961

Citizenship: U.S.A.

Employment

January 2000-
present 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

July 1993-
July 1995 Yale University, Clare Boothe Luce Associate Professor
of Applied Physics and Physics

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

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 Ba₂YCu₃O_{7-x}: 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 Ba₂YCu₃O_{7-x} 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 Ba₂YCu₃O_{7-x}", 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 O₄," 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 C₆₀," 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 BaTiO₃ 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 K₄ C₆₀," 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 BaTiO₃" 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 *Proceedings 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}C₆₀," 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 PbTiO₃ 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 PbZrO₃ 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 Al₂Ru 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 $\text{Yb}_{2.75}\text{C}_{60}$," 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).
46. "Dynamic local distortions in ferroelectrics," H. Krakauer, R. Yu, C.Z. Wang, K.M. Rabe and U.V. Waghmare, *J.Phys. Cond. Matt.* **11**, 3779 (1999).
47. "Effective Hamiltonian for the ferroelectric phase transitions in KNbO_3 ," U. V. Waghmare, K. M. Rabe, H. Krakauer, R. Yu and C.-Z. Wang, in *First-Principles Calculations for Ferroelectrics*, ed. by R. E. Cohen, AIP Conference Proceedings 436 (American Institute of Physics, Woodbury, New York, 1998).
48. "Temperature-dependent dielectric and piezoelectric response of ferroelectrics from first principles," K. M. Rabe and E. Cockayne, in *First-Principles Calculations for Ferroelectrics*, ed. by R. E. Cohen, AIP Conference Proceedings 436 (American Institute of Physics, Woodbury, New York, 1998).
49. "Configuration dependence of physical properties of a ferroelectric solid solution," E. Cockayne and K. M. Rabe, in *First-Principles Calculations for Ferroelectrics*, ed. by R. E. Cohen, AIP Conference Proceedings 436 (American Institute of Physics, Woodbury, New York, 1998).
50. "The local structure of ferroelectric $\text{Pb}_{1-x}\text{Ge}_x\text{Te}$," B. Ravel, E. Cockayne and K. M. Rabe, *J. Synchrotron Rad.* **6**, 567 (1999).
51. "First-principles investigation of ferromagnetism and ferroelectricity in bismuth manganite," N. A. Hill and K. M. Rabe, *Phys. Rev.* **B59**, 8759 (1999).
52. "Combined EXAFS and first-principles theory study of $\text{Pb}_{1-x}\text{Ge}_x\text{Te}$," B. Ravel, E. Cockayne, M. Newville and K. M. Rabe, *Phys. Rev.* **B60**, 14632 (1999).
52. "Ferroelectricity in PbTiO_3 thin films: a first-principles approach," Ph. Ghosez and K. M. Rabe, *J.Electroceram.* **4**, 379 (2000).
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).
54. "Pressure dependence of instabilities in perovskite PbZrO_3 ," E. Cockayne and K. M. Rabe, *J. Phys. Chem. Solids* **61**, 305 (2000).
55. "First-principles study of lattice instabilities in $\text{Ba}_x\text{Sr}_{1-x}\text{TiO}_3$," Ph. Ghosez, D. Desquesnes, X. Gonze and K. M. Rabe, in "Fundamental Physics of Ferroelectrics 2000," ed. by R. E. Cohen, AIP Conference Proceedings 535, (American Institute of Physics, Woodbury, New York, 2000).

56. "A microscopic model of ferroelectricity in stress-free PbTiO_3 ultrathin films," Ph. Ghosez and K. M. Rabe, *Appl. Phys. Lett.* **76**, 2767 (2000).
57. "Soft tetragonal distortions in ferromagnetic Ni_2MnGa and related materials from first principles," V. Godlevsky and K. M. Rabe, *Phys. Rev. B* **63**, 134407 (2001).
58. Xiangyang Huang, Claudia Bungaro, Vitaliy Godlevsky and Karin M. Rabe, "Lattice instabilities of cubic NiTi from first principles," *Phys. Rev. B* **65**, 014108 (2002).
59. C. Bungaro and K. M. Rabe, "Lattice instabilities of $\text{PbZrO}_3/\text{PbZrO}_3$ [1:1] superlattices from first principles," *Phys. Rev. B* **65**, 224106 (2002).
60. N. Sai, K. M. Rabe and D. Vanderbilt, "Theory of structural response to macroscopic electric fields in ferroelectric systems," *Phys. Rev. B* **66**, 104108 (2002).
61. J. B. Neaton, C. L. Hsueh and K. M. Rabe, "Enhanced polarization in strained BaTiO_3 from first principles," *MRS Proceedings Vol. 718*, ed. by K. Poepelmeier, A. Navrotsky and R. Wentzcovitch (2002).
62. K. M. Rabe, "Tunability of high-dielectric-constant materials from first principles," *MRS Proceedings Vol. 718*, ed. by K. Poepelmeier, A. Navrotsky and R. Wentzcovitch (2002).
63. X. Huang, K. M. Rabe and G. J. Ackland, "First-principles study of the structural energetics of PdTi and PtTi ," *Phys. Rev. B* **67**, 024101 (2003).
64. Karin M. Rabe, "Book Review: Band Theory and Electronic Properties of Solids," *Physics Today*, December 2002, pp.61-62.
65. J. B. Neaton and K. M. Rabe, "Theory of polarization enhancement in epitaxial $\text{BaTiO}_3/\text{SrTiO}_3$ superlattices," *Appl. Phys. Lett.* **82**, 1586 (2003).
66. Hao Li, H. Zheng, L. Salamanca-Riba, R. Ramesh, I. Naumov, and K. Rabe, "Origin of antiphase domain boundaries and their effect on the dielectric constant of $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{TiO}_3$ films grown on MgO substrates," *Appl. Phys. Lett.* **81**, 4398 (2002).
67. K. M. Rabe, "News and Views: Think locally, act globally," *Nature Materials* **1**, 147 (2002).
68. S. Tinte, J. Iniguez, K. M. Rabe and D. Vanderbilt, "Quantitative analysis of the first-principles effective Hamiltonian approach to ferroelectric perovskites," *Phys. Rev. B* **67**, 064106 (2003).
69. K. M. Rabe, "Lattice instabilities of complex perovskite oxides from first principles," *Computer Simulation Studies in Condensed Matter Physics XVI*, Springer Proceedings in Physics, in press.
70. X. Huang, G. J. Ackland, K. M. Rabe, "Crystal structures and shape-memory behaviour of NiTi ," *Nature Materials* **2**, 307 (2003).
71. J. Wang, J. B. Neaton, H. Zheng, V. Nagarajan, S. B. Ogale, B. Liu, D. Viehland, V. Vaithyanathan, D. G. Schlom, U. V. Waghmare, N. A. Spaldin, K. M. Rabe, M. Wuttig, and R. Ramesh, "Epitaxial BiFeO_3 multiferroic thin film heterostructures," *Science* **299**, 1719 (2003).

72. C. Bungaro, K. M. Rabe and A. Dal Corso, "First-principles study of lattice instabilities in ferromagnetic Ni_2MnGa ," *Phys. Rev. B* 68, 134104 (2003).
73. S. Tinte, K. M. Rabe and D. Vanderbilt, "Anomalous enhancement of tetragonality in PbTiO_3 induced by negative pressure," *Phys. Rev. B* 68, 144105 (2003).
74. G. J. Ackland, X. Y. Huang and K. M. Rabe, "First-principles thermodynamics of transition metals: W, NiAl, and PdTi," *Phys. Rev. B* 68, 214104 (2003)
75. C. J. Fennie and K. M. Rabe, "Structural and dielectric properties of Sr_2TiO_4 from first principles," *Phys. Rev. B* 68, 184111 (2004).
76. O. Dieguez, S. Tinte, A. Antons, C. Bungaro, J. B. Neaton, K. M. Rabe and D. Vanderbilt, "Ab initio study of the phase diagram of epitaxial BaTiO_3 ," *Phys. Rev. B* 69, 212101 (2004).
77. C. Bungaro and K. M. Rabe, "Epitaxially strained $[\text{001}](\text{PbTiO}_3)_1(\text{PbZrO}_3)_1$ superlattice and PbTiO_3 from first principles," *Phys. Rev. B* 69, 184101 (2004).
78. C. H. Ahn, K. M. Rabe and J. M. Triscone, "Ferroelectricity at the nanoscale: Local polarization in oxide thin films and heterostructures," *Science* 303, 488 (2004).
79. J. W. Reiner, F. J. Walker, R. A. McKee, C. A. Billman, J. Junquera, K. M. Rabe and C. H. Ahn, "Ferroelectric stability of BaTiO_3 in a crystalline oxide on semiconductor structure," *Phys. Stat. Sol. B* 241, 2287-2290 (2004).
80. X. Y. Huang, I. I. Naumov and K. M. Rabe, "Phonon anomalies and elastic constants of cubic NiAl from first principles," *Phys. Rev. B* 70, 064301 (2004).
81. C. Bungaro and K. M. Rabe, "Coexistence of antiferrodistortive and ferroelectric distortions at the $\text{PbTiO}_3(001)$ surface," *Phys. Rev. B* 71, 035420 (2005).
82. D. R. Hamann, X. F. Wu, K. M. Rabe and D. Vanderbilt, "Metric tensor formulation of strain in density-functional perturbation theory," *Phys. Rev. B* 71, 035117 (2005).
83. D. R. Hamann, X. F. Wu, K. M. Rabe and D. Vanderbilt, "Generalized-gradient-functional treatment of strain in density-functional perturbation theory," *Phys. Rev. B* 72, 033102 (2005).
84. C. J. Fennie and K. M. Rabe, "First principles investigation of ferroelectricity in epitaxially strained Pb_2TiO_4 ," *Phys. Rev. B* 71, 100102 (2005).
85. A. Antons, J. B. Neaton, K. M. Rabe and D. Vanderbilt, "Tunability of the dielectric response of epitaxially strained SrTiO_3 from first principles," *Phys. Rev. B* 71, 024102 (2005).
86. J. B. Neaton, C. Ederer, U. V. Waghmare, N. A. Spaldin and K. M. Rabe, "First principles study of spontaneous polarization in multiferroic BiFeO_3 ," *Phys. Rev. B* 71, 014113 (2005).
87. K. Johnston, X. Y. Huang, J. B. Neaton and K. M. Rabe, "First-principles study of symmetry lowering and polarization in $\text{BaTiO}_3/\text{SrTiO}_3$ superlattices with in-plane expansion," *Phys. Rev. B* 71, 100103 (2005).

88. M. Dawber, K. M. Rabe and J. F. Scott, "Physics of thin-film ferroelectric oxides," *Rev. Mod. Phys.* 77, 1083 (2005).
89. C. J. Fennie and K. M. Rabe, "Ferroelectric transition in YMnO_3 from first principles," *Phys. Rev. B* 72, 100103 (2005).
90. S. M. Nakhmanson, K. M. Rabe and D. Vanderbilt, "Polarization enhancement in two- and three-component ferroelectric superlattices," *Appl. Phys. Lett.* 87, 102906 (2005).
91. M. Dawber, C. Lichtensteiger, M. Cantoni, M. Veithen, Ph. Ghosez, K. Johnston, K. M. Rabe and J. M. Triscone, "Unusual behavior of the ferroelectric polarization in $\text{PbTiO}_3/\text{SrTiO}_3$ superlattices," *Phys. Rev. Lett.* 95, 177601 (2005).
92. A. T. Zayak, P. Entel, K. M. Rabe, W. A. Adeagbo and M. Acet, "Anomalous vibrational effects in non-magnetic and magnetic Heusler alloys," *Phys. Rev. B* 72, 054113 (2005).
93. A. T. Zayak, W. A. Adeagbo, P. Entel and K. M. Rabe, "e/a dependence of the lattice instability of cubic Heusler alloys from first principles," *Appl. Phys. Lett.* 88, 111903 (2006)
94. O. Dieguez, K. M. Rabe and D. Vanderbilt, "First principles study of epitaxial strain in perovskites," *Phys. Rev. B* 72, 144101 (2005).
95. A. Posadas, J. B. Yan, J. Han, C. H. Ahn, S. Gariglio, K. Johnston, J. B. Neaton and K. M. Rabe, "Epitaxial growth of multiferroic YMnO_3 on GaN," *Appl. Phys. Lett.* 87, 171915 (2005).
96. C. J. Fennie and K. M. Rabe, "Polar phonons and intrinsic dielectric response of the ferromagnetic insulating spinel CdCr_2S_4 from first principles," *Phys. Rev. B* 72, 214123 (2005).
97. S. M. Nakhmanson, K. M. Rabe and D. Vanderbilt, "Predicting polarization enhancement in multicomponent ferroelectric superlattices," *Phys. Rev. B* 73, 060101 (2006).
98. C. J. Fennie and K. M. Rabe, "Magnetic-induced phonon anisotropy in ZnCr_2O_4 from first principles," *Phys. Rev. Lett.*, in press
99. C. J. Fennie and K. M. Rabe, "Ferroelectricity in the Dion-Jacobson $\text{CsBiNb}_2\text{O}_7$ from first principles," *Appl. Phys. Lett.*, in press.
100. T. Thonhauser and K. M. Rabe, "fcc breathing instability in BaBiO_3 from first principles," *cond-mat/0507377*.
101. A. T. Zayak, X. Huang, J. B. Neaton and K. M. Rabe, "Structural, electronic and magnetic properties of SrRuO_3 under epitaxial strain," *cond-mat/0605606*.

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 $\text{Pb}_{1-x}\text{Ge}_x\text{Te}$," 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 $\text{Pb}_{0.75}\text{Ge}_{0.25}\text{Te}$," 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," 5th 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.

Recent Departmental Colloquia

1. "Ferroelectrics by Design," Materials Department Colloquium, U. California at Santa Barbara, October 2005
2. "Designer Oxides that Work," Distinguished Women in Physics Lecture/Physics Department Colloquium, U. Texas at Austin, March 2006.
3. "Designer Oxides that Work," Physics Department Colloquium, Yale University, April 2006.

PhD Students Supervised

Serdar Ogut, PhD in Physics, Yale University, 1995. Upon graduation, obtained postdoctoral position at the University of Minnesota. Currently Associate 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 Research Scientist at J. Nehru Research Centre, Bangalore, India.

Craig J. Fennie, current student in PhD program in Physics at Rutgers University. Degree expected summer 2006; position as the Nicholas Metropolis Fellow in Computational Physics at Argonne National Laboratory begins 1 October 2006.

Carl-Johann Eklund, current student in PhD program in Physics at Rutgers University.

Postdoctoral fellows supervised

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

Nicola Hill (now Spaldin) 1996; current position: Associate Professor of Materials, University of California, Santa Barbara

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.

Claudia Bungaro 2000-2004

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

Ivan I. Naumov 2001-2003; current position: postdoctoral research fellow, University of Arkansas.

Silvia Tinte (co-supervised with D. Vanderbilt) 2001-2004; current position: postdoctoral research fellow, NIST.

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

Karen Johnston, 2003-2005, current position: postdoctoral research fellow, University of Helsinki

Alexey Zayak, 2004-present

Serge Nakhmanson (co-supervised with D. Vanderbilt) 2004-present

Timo Thonhauser (co-supervised with D. Vanderbilt and D. Langreth) 2004-present

Shen Li (co-supervised with D. Langreth) 2005-present

Valentino Cooper (co-supervised with D. Langreth) 2005-present

Grant support

“First-principles effective Hamiltonians for high-performance ferroelectrics and piezoelectrics,” ONR, \$482,185, 2/1/2001-12/31/2004; annual average \$123,111.

Materials Research Science and Engineering Center, NSF/University of Maryland \$1,021,996 (3 P.I.'s), 9/1/2000-8/31/2005; annual average roughly \$75,000.

“A virtual laboratory for first-principles design of piezoelectrics for transducers,” ONR/College of William and Mary, \$568,626 (research conducted in collaboration with David Vanderbilt), 2/1/2001-1/31/2005; annual average \$142,157.

“Computational tools for the atomistic-continuum interface: nanometer-to-millimeter scale aircraft,” AFOSR/ University of Minnesota, \$314,533, 6/1/2001-5/31/2003; annual average \$104,844.

“Artificially structured nanoscale ferroelectrics,” NSF/Pennsylvania State University, \$239,997, 5/1/2001-4/30/2005, annual average \$60,000.

“The nanoscale materials physics of epitaxial ferroelectric oxide systems,” DOE/Yale : \$317,137, 9/15/2001-3/14/2005, annual average \$90,611.

“Acquisition of a network cluster of advanced workstations for first principles calculations of the electronic structure of complex materials,” NSF (MRI) \$320,083 (with G. Kotliar, D. Vanderbilt and C. Uebing), 9/1/2001-8/31/2003.

Professional activities since 2000

Aspen Center for Physics: General Member (since 1995), Scientific Secretary (2000-2001), Trustee (since 2002).

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.

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

Co-organizer (with D. Vanderbilt and K. Burke), 16th Annual Workshop on Recent Developments in Electronic Structure Methods, Rutgers University, Piscataway, New Jersey, May 2004.

Co-organizer (with R. Ramesh) of Division of Materials Physics focused session “Polarization in ferroelectric thin films,” American Physical Society March meeting 2001.

Co-organizer (with R. E. Cohen), Aspen Center for Physics Winter Conference “Fundamental Physics of Ferroelectrics,” Aspen, Colorado, February 2000.

David Adler Lectureship Award committee, American Physical Society: member 2003, chair 2004.

Division of Materials Physics Fellowship Committee, American Physical Society, 2005, 2006.

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

Editorial Board, Physical Review B, 2003-present.

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

Panelist: Information Technology Research Medium Materials panel, National Science Foundation, April 2003

High Performance Computing Modernization Office Challenge Board member (annual evaluation of Challenge Projects for the Department of Defense), through 2002.

K-12 Outreach

Assistant in “buckyball” program for grade school students, U. California at Santa Barbara, spring 2001
Instructor of “buckyball” program for high school girls through the Douglass Project, Rutgers University (Douglass Science Institute, June 2002, Douglass Weekend Science Academy, Fall 2001, 2002 and 2003)

Significant Rutgers University activities

A&P Committee, 2004-2005.

FASIP Peer Evaluation Committee, academic year 2002-2003

Packard Fellowship Selection Committee (including assisting nominees with preparation of applications)
2002, 2003

Physics Department Graduate Oral Examination committee: Fall 2001—Spring 2003.

Physics Department building committee and office assignments for condensed matter theory group, since
Fall 2002.

Rutgers University Teaching

Physics 272 (recitations), Honors Physics II, Spring 2000

Physics 601, Solid State Physics I; Fall 2000, Fall 2001, Fall 2002, Fall 2003, Fall 2004

Physics 602, Solid State Physics II; Spring 2002, Spring 2003, Spring 2004

Physics 627 (series of three lectures), Surface Science, Fall 2002

Physics 140, The Greenhouse Effect, Spring 2005, Spring 2006