Kathie E. Newman

CONTACT INFORMATION

Department of Physics
University of Notre Dame
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CITIZENSHIP

United States

RESEARCH INTERESTS

Complex Materials: Clusters, Alloys, Liquids, Compounds; Statistical Mechanics: Phase Transitions, Ordering, Simulations; Model Building and Method Development: Ice, Multipoles in Molecular Dynamics

EDUCATION

University of Washington, Seattle, Washington

Ph.D., Department of Physics, December 1981

Thesis Title: "The Scaling-Field Formulation of the Wilson Equation and its Application to Critical Phenomena"
Adviser: Professor Eberhard K. Riedel
Area of Study: Renormalization-Group Theory and Critical Phenomena

Michigan State University, E. Lansing, Michigan

B.S., Department of Physics and Astronomy, June 1974

ACADEMIC APPOINTMENTS

Professor July 1987-present
Department of Physics, University of Notre Dame

Director of Graduate Graduate Admissions July 2008 to June 2014
Department of Physics, University of Notre Dame

Director of Graduate Studies July 2003 to June 2012
Department of Physics, University of Notre Dame

Associate Chair of Physics July 2003 to June 2012
Department of Physics, University of Notre Dame

Associate Dean August 1987 to June 2002
College of Science, University of Notre Dame

Associate Professor July 1987 to June 1994
Department of Physics, University of Notre Dame

Assistant Professor September 1983 to June 1987
Department of Physics, University of Notre Dame

Research Assistant Professor August 1983 to September 1983
Department of Physics, University of Illinois at Urbana-Champaign

Postdoctoral Research Associate November 1981 to August 1983
Department of Physics, University of Illinois at Urbana-Champaign

Refereed Journal Publications

M. Lamichhane, J. D. Gezelter, and K.E. Newman, "Real Space Electrostatics for Multipoles: I. Development of Methods," J. Chem. Phys. **141**, 134109 (2014).

M. Lamichhane, K.E. Newman, and J. D. Gezelter, "Real Space Electrostatics for Multipole. II. Comparisons with the Ewald Sum," J. Chem. Phys. **141**, 134110 (2014).

H. A. Fox, K. E. Newman, W. F. Schneider, and S. A. Corcelli, "Bulk and Surface Properties of Rutile TiO_2 from Self-Consistent-Charge Density Functional Tight Binding," J. Chem. Theory Comput. **6**, 499-507 (2010).

E.M. Vandeworp and K.E. Newman, "Coherent Alloy Phase Separation: Differences in Canonical and Grand Canonical Ensembles," Phys. Rev. B**55**, 14222-14229 (1997).

M.R. Weidmann and K.E. Newman, "Effects of Site Correlations on the Local Structure of Strain-Relaxed Semiconductor Alloys," Phys. Rev. B**51**, 4962-4981 (1995).

E.M. Vandeworp and K.E. Newman, "Order-Disorder on a Model Lattice Midmatched Binary Alloy," Phys. Rev. B**52**, 4086-4092 (1995).

K.M. Kemner, B.A. Bunker, H. Luo, N. Samarth, J.K. Furdyna, M.R. Weidmann, and K.E. Newman, "Atomic rearrangement at interfaces in ZnTe/CdSe superlattices," Phys. Rev. B**50**, 14327-14335 (1994).

K.E. Newman, T. Kim, and X.O. Xiang, "Ground States and Ordering in Semiconducting (Chalcopyrite)-(Zinc-Blende) Alloys," *Statics and Dynamics of Alloy Phase Transitions*, P.E.A. Turchi and A. Gonis, Eds., 553-556 (Plenum, NY, 1993).

K.M. Kemner, B.A. Bunker, H. Luo, N. Samarth, J.K. Furdyna, M.R. Weidmann, and K.E. Newman, "X-Ray Absorption Spectroscopy Investigations of Atomic Reordering at ZnTe/CdSe Interfaces," *Statics and Dynamics of Alloy Phase Transformations*, P.E.A. Turchi and A. Gonis, Eds., 203-206 (Plenum, NY, 1993).

K.M. Kemner, B.A. Bunker, H. Luo, N. Samarth, J.K. Furdyna, M.R. Weidmann, and K.E. Newman, "EXAFS Studies of Interfaces in ZnTe/CdSe Superlattices," Jpn. J. Appl. Phys. **32**, 399-403 (1992).

R.J. Cohen and K.E. Newman, "Commensurate and Incommensurate Phases of Epitaxial Semiconductor Antiferromagnets with 'Built-In′ Strain," Phys. Rev. B**46** (Rapid Commun.) 14282-14285 (1992).

K.M. Kemner, B.A. Bunker, H. Luo, N. Samarth, J.K. Furdyna, M.R. Weidmann, K.E. Newman, "Extended X-Ray-Absorption Fine-Structure Studies of Interfaces in ZnTe/CdSe Superlattices," Phys. Rev. B**46** (Rapid Commun.), 7272-7275 (1992).

M.R. Weidmann, J.R. Gregg and K.E. Newman, "Local Structure of $Zn_{1-x}Mn_xSe$ Alloys," Journal of Physics: Condensed Matter **4**, 1895-1904 (1992).

M.R. Weidmann and K.E. Newman, "Simulation of Elastic Network Relaxation: The $Si_{1-x}Ge_x$ Random Alloy," Phys. Rev. B**45**, 8388-8396 (1992).

K.E. Newman and X.O. Xiang, "Demonstration of Ordering in Semiconducting (Chalcopyrite)-(Zinc-Blende) Alloys," Phys. Rev. B**44** (Rapid Commun.), 4677-4679 (1991).

D. Teng, J. Shen, K.E. Newman, and B.-L. Gu, "Effects of Ordering on the Band Structure of III-V Semiconductors," J. Phys. Chem. Solids **52**, 1109-1128 (1991).

M.-H. Tsai, J.D. Dow, K.E. Newman, and R.V. Kasowski, "Theory of Local Bond-Length Relaxation in $Hg_{1-x}Cd_xTe$ Alloys," Phys. Rev. B**41**, 7744-7748 (1990).

K.E. Newman, J.D. Dow, B.A. Bunker, L.L. Abels, P.M. Raccah, S. Ugur, D.Z. Xue, and A. Kobayashi, "Effects of a zinc-blende-diamond order-disorder transition on the crystal, electronic, and vibrational structures of metastable $(GaAs)_{1-x}(Ge_2)_x$ alloys," Phys. Rev. B**39**, 657-662 (1989).

K.E. Newman, J. Shen, and D. Teng, "Effects of Strain on Structural Properties in Ordered Semiconductors," Superlattices and Microstructures **6**, 245-257 (1989).

B.L. Gu, K.E. Newman, P.A. Fedders, "Role of Correlations in $(GaSb)_{1-x}Ge_{2x}$ Alloys," Phys. Rev. B**35**, 9135-9148 (1987).

A. Kobayashi, K.E. Newman, and J.D. Dow, "Densities of Phonon States for $(GaSb)_{1-x}Ge_{2x}$," Phys. Rev. B**32**, 5312-5327 (1985).

K.E. Newman, J.D. Dow, A. Kobayashi, and R. Beserman, "Explanation of the Anomalous Raman Spectra of $(GaSb)_{1-x}Ge_{2x}$," Solid State Commun. **56**, 556 (1985).

K.E. Newman and D.W. Jenkins, "Metastable (III-V)$_{2x}$IV$_{2x}$ Alloys," Superlattices and Microstructures, **1**, 275-278 (1985).

D.W. Jenkins, K.E. Newman, and J.D. Dow, "Predicted Energy Bands Gaps of $A_x^{III}B_{1-x}^{V}$ Metastable, Substitutional, Crystalline Alloys," Phys. Rev. B**32**, 4034-4041 (1985).

E.K. Riedel, G.R. Golner, and K.E. Newman, "Scaling-Field Representation of Wilsons Exact Renormalization-Group Equation," Am. Phys. (NY) **161**, 178-238 (1985).

K.E. Newman and J.D. Dow, "Core Excitons in Si_xGe_{1-x} Alloys," Solid State Commun. **50**, 587 588 (1984).

K.E. Newman and E.K. Riedel, "Critical Exponents by the Scaling-Field Method: The Isotropic N-Vector Model in Three Dimensions," Phys. Rev. B**30**, 6615-6638 (1984).

S.F. Ren, K.E. Newman, J.D. Dow, and O.F. Sankey, "Energy levels of paired donor impurities in Si_xGe_{1-x} alloys," Appl. Phys. **A101**, 269-272 (1984).

D.W. Jenkins, K.E. Newman, and J.D. Dow, "Metastable $(InP)_{1-x}Ge_{2x}$ alloys as potential materials with band gap of $\sim$10 μm," J. Appl. Phys. **55**, 3871-3872 (1984).

K.E. Newman, E.K. Riedel, and S. Muto, "Q-state Potts Model by Wilson′s Exact Renormalization-Group Equation," Phys. Rev. B**29**, 302-313 (1984).

K.E. Newman and J.D. Dow, "Theory of deep impurities in silicon-germanium alloys," Phys. Rev. B**30**, 1929-1936 (1984).

K.E. Newman and J.D. Dow, "A new type of order-disorder transition in metastable $(GaAs)_{1-x}Ge_{2x}$ Alloys," J. Vac. Sci. and Tech. B**1**, 243-245 (1983).

K.E. Newman and J.D. Dow, "Bifurcation of deep impurities in metastable $(GaAs)_{1-x}Ge_{2x}$ alloys," Appl. Phys. Lett. **42**, 1033-1035 (1983).

M.A. Bowen, A.C. Redfield, D.V. Froelich, K.E. Newman, R.E. Allen, and J.D. Dow "Effects of an order-disorder transition on surface deep levels in metastable $(GaAs)_{1-x}Ge_{2x}$," J. Vac. Sci. and Tech. B**1**, 747-750 (1983).

B.R. Tittmann, E. Domany, J.L. Opsal and K.E. Newman "Elastic wave scattering from irregular voids," J. Appl. Phys. **54**, 6079-6085 (1983).

K.E. Newman, A. Lastras-Martinez, B.Kramer, S.A. Barnett, M.A. Ray, J.D. Dow, J.E. Greene, and P.M. Raccah, "Optical Absorption in Single-Crystal Metastable $(GaAs)_{1-x}Ge_{2x}$ Alloys: Evidence for a Zincblende-Diamond Order-Disorder Transition," Phys. Rev. Lett. **50**, 1466-1469 (1983).

A.C. Redfield, M.A. Bowen, K.E. Newman, and J.D. Dow, "Surface States of Metastable $(GaAs)_{1-x}Ge_{2x}$ Alloys," Solid State Commun. **46**, 371-373 (1983).

K.E. Newman and J.D. Dow, "Zincblende-diamond order-disorder transition in metastable crystal-line $(GaAs)_{1-x}Ge_{2x}$ Alloys," Phys. Rev. B**27**, 7495-7508 (1983).

K.E. Newman and E.K. Riedel, "Cubic N-Vector model and randomly dilute Ising model in general dimensions," Phys. Rev. B**25**, 264-280 (1982).

K.E. Newman, S. Teitel, and E. Domany, "The Distorted Wave Born Approximation: Application to Elastodynamics," J. Appl. Phys. **52**, 4363-4370 (1981).

G.R. Golner, K.E. Newman, and E.K. Riedel, "Solution of the Exact Wilson Renormalization-Group Equation by the Scaling-Field Method," J. Appl. Phys. **49**, 1359-1359 (1978).

Referred Conference Publications

K.E. Newman, D. Teng, J. Shen, and B.-L. Gu, "Effects of Ordering in Ternary Semiconductor Alloys: Electronic and Structural Properties," *Band Structure Engineering in Semiconductors,* Ed. R.A. Abram and M. Jaros, 119-127 Plenum, NY (1989).

K.E. Newman, J. Shen, D. Teng, B.-L. Gu, S.-Y. Ren, and J.D. Dow, "Electronic and Structural Properties of Ordered III-V Alloys," *Alloy Phase Stability*, Eds. G.M. Stocks and A. Gonis, 621 625, Kluwer, Dordrecht (1989).

K.E. Newman, B.L.Gu, and P.A. Fedders, "Correlations and Ordering in $(GaSb)_{1-x}Ge_{2x}$ Alloys," *Proceedings of the 1986 MRS Fall Meeting*, **77**, (1987), J.D. Dow and I.K. Schuller, p.59-70 (Materials Research Society, Pittsburgh, 1987).

K.E. Newman, "Consequences of the Zincblende-Diamond Order-Disorder Transition for $(GaAs)_{1-x}Ge_{2x}$ and Other Alloys," *Proceedings of the 17th International Conference on the Physics of Semiconductors*, ed. J.D. Chadi and W.A. Harrison, Springer-Verlag, pp. 955-960 (1985).

E.K. Riedel and K.E. Newman, "Critical Phenomena from Wilson′s Exact Renormalization-Group Equation," *Statics and Dynamics of Nonlinear Systems*, ed. G. Benedek, H. Bilz, and R. Zeyer (Springer, Berlin, 1983) p. 80-85.

E.K. Riedel and K.E. Newman, "Scaling-Field Approach to Critical Phenomena," *Magnetic Phase Transitions*, ed. M. Ausloos and R.J. Elliott (Springer, Berlin, 1983) p. 76-80.

E. Domany, K.E. Newman, and S. Teitel, "Elastic Wave Scattering by General Shaped Defects: The Distorted Wave Born Approximation," *Proceedings of the ARPA/AFML Review of Progress in Quantitative NDE*, ed. D.O. Thompson, AFWAL-TR-80-4078, 341-346 (1980).

E. Domany and K.E. Newman, "Calculation of Scattering by the Distorted Wave Born Approximation," *Proceedings of the ARPA/AFML Review of Progress in Quantitative NDE*, ed. D.O. Thompson, AFML-TR-78-205, 404 (1979).

In Process

D.M. McDermott and K.E. Newman, "Wade's Rules and the Stability of Au_nGe_m Clusters," Accepted by *EPJD* on Feb. 4, 2015.

Invited Addresses

"Physics Graduate Students: Assess the Program or the Individual?" 2013 AAPT Summer meeting in Portland, Oregon, 7/16/13

"Coherent Alloy Phase Separation: Differences in Canonical and Grand Canonical Ensembles," CECAM Workshop on Theoretical Predictions of Alloy Phase Stability, Lyon, France, June 11, 1996.

"Structural and Electronic Properties of Ordered Semiconductors," 1989 Electronic Materials Conference, M.I.T., Cambridge, Massachusetts, June 22, 1989.

"Effects of Ordering in Semiconductor Alloys: Electronic and Structural Properties," Keynote Address, NATO Advanced Research Workshop on Band Structure Engineering in Semiconductor Microstructures at Il Ciocco, Lucca, Italy, April 12, 1988.

"Ordering Transitions in Alloys," Workshop on the Physical and Mechanical Properties of Alloys: Semiconductors and Beyond, Dayton, Ohio, September 29, 1987.

"Ordering Transitions in Semiconductors," Materials Research Society meeting, December 6, 1986, Boston.

"Metastable $(\mathrm{III\ V})_{1-x}\mathrm{IV}_{2x}$ Alloys," First International Conference on Superlattices, Microstructures, and Microdevices, August 13, 1984, Champaign, Illinois.

"Consequences of the Zincblende-Diamond Order-Disorder Transition for $(\mathrm{GaAs})_{1-x}\mathrm{Ge}_{2x}$ and Other Alloys," 17th International Conference on the Physics of Semiconductors, August 8, 1984, San Francisco.

"Theory of Zincblende-Diamond Order-Disorder Phase Transition in Metastable $(\mathrm{GaAs})_{1-x}\mathrm{Ge}_{2x}$ Alloys," March Meeting of the American Physical Society, March 26, 1984, Detroit, Michigan.

"Electronic Effects of an Order-Disorder Zincblende-Diamond Phase Transition in Metastable $(\mathrm{GaAs})_{1-x}\mathrm{Ge}_{2x}$Alloys," Midwest Solid-State Theory Symposium, Cleveland, Ohio, October 18, 1983.

Invited Seminars and Colloquia

"Lessons on Climate and Curriculum for Physics," Colloquium, University of Nebraska, February 20, 2008.

"Global Strain Relaxation in Non-Random Semiconductor Alloys," Colloquium, Illinois State University, April 3, 1995.

"Global Strain Relaxation in Non-Random Semiconductor Alloys," Seminar, Ohio State University, Febuary 27, 1995.

"Global Strain Relaxation in Non-Random Semiconductor Alloys," Colloquium, Michigan Technological University, March, 1993.

"Studies of Local Structure and its Effects in Semiconductors," Seminar, Michigan State University, July 11, 1991.

"The Effects of Ordering in Semiconductor Alloys," Seminar, Purdue University, September 29, 1989.

"Order Disorder Transitions in Semiconductors," Seminar, University of Science andTechnology of China, Hefei, Anhui Province, PRC, May 26, 1987.

"Deep Traps in Silicon Germanium Alloys" and "Renormalization Group Theory and Critical Phenomena," four lectures, Tsinghua University, Beijing, PRC, May 15 to May 21, 1987.

"Order Disorder Transitions in Semiconductors," Seminar, Tsinghua University, Beijing, PRC, May 14, 1987.

"Ordering Transitions in Semiconductors," Seminar, University of Pittsburgh, March 5, 1987.

"Ordering Transitions in Semiconductors," Colloquium, Western Michigan University, October 14, 1986.

"Phase Transitions and Correlations in (GaAs)-Ge and Related Alloys," Seminar, Purdue University, February 10, 1986.

Awards

University of Notre Dame

Director of Graduate Studies Award	2013
Kaneb Center Teaching Award	2005
Special Presidential Award	1999
Special Presidential Award	1996

Selected Service Activities

Graduate Students

Family Friendly Policies workgroup of the Graduate School, 2010-2011
Report: Creating a more Family-Friendly Environment for Graduate Students

Physics

Site Visits: *Improving the Climate for Women*, Committee on the Status of Women in Physics

- Harvard (1994)
- Purdue (2003)
- U. of Michigan (2005)
- Indiana University, Bloomington (2007)
- NSCL, Michigan State University (2009).

Site Visits: *Strategic Programs for Innovations in Undergraduate Physics* (SPINUP)

- U. of Illinois, Urbana-Champaign (2001)
- Lawrence University (2002)

Associate Dean Activities

Undergraduate Affairs

- Advised undergraduates on majors
- Oversaw degree integrity
- Worked with Prof. Steven Buechler on developing degree audit program
- Chaired College of Science Curriculum Committee
- Cooperative Council for Teacher Education (1993-2002)
- Notre Dame/Saint Marys College Liaison for Teacher Education (1991-2002)

Planning Committees for Jordan Hall of Science (1993-2002)

Computing

- Chaired College of Science Computing Committee
- Chaired Committee on Technical Computing
- Developed and directed Science Computing Facilities (1995-2002)

Teaching

Courses Developed and Taught

PHYS 20451, Mathematical Methods in Physics I
PHYS 532 (old system), Renormalization-Group Theory
PHYS 70500, Introduction to Condensed Matter Physics
PHYS 77031, Review of Fundamental Physics I
PHYS 77032, Review of Fundamental Physics II
PHYS 80502, Soft Condensed Matter Physics
PHYS 95000, Teaching Practicum

Undergraduate Courses Taught

PHYS 116 (old system), Principals of Physics II
PHYS 127 (old system), General Physics I
PHYS 251 (old system), Mechanics I
PHYS 252 (old system), Mechanics II
PHYS 20454, Intermediate Mechanics
PHYS 356 (old system) Electricity and Magnetism I
PHYS 30421, Scientific Programming
PHYS 43411, Senior Seminar

Graduate Courses Taught

PHYS 70003, Mathematical Methods in Physics
PHYS 70005, Classical Mechanics
PHYS 70006, Electromagnetism
PHYS 80001, Electrodynamics
PHYS 80002, Statistical Thermodynamics
PHYS 80501, Solid State Physics
PHYS 614 (old system), Solid State Physics II

Dissertations Supervised

Ph.D., Danielle M. McDermott, 2014

Directors: Kathie E. Newman and Cynthia J. Olson Reichhardt
"Pattern Formation in Micro and Nano Systems"

Ph.D., Laura K. Kinnaman, 2012

Directors: Kathie E. Newman and Steven A. Corcelli
"Structural, dynamic, and spectroscopic properties of self-consistent charge density functional tight binding water models"

Ph.D., Seng Kai Wong, 2005

Directors: Kathie E. Newman and James A. Glazier
"A Cursory Study of the Thermodynamic and Mechanical Properties of Monte-Carlo Simulations of the Ising Model"

Ph.D., Taek H. Kim, 2003

Director: Kathie E. Newman
"Structural and Thermodynamic Properties of Quaternary Semiconductor Alloys"

Ph.D.,Evert M. Vandeworp, 1996

Director: Kathie E. Newman
"Effect of Elastic Interactions on the Phase Stability of Lattice-Mismatched Alloys"

Ph.D., Matthew R. Weidmann, 1992

Director: Kathie E. Newman
"Global Strain Relaxation in Random, Ordered, and Correlated Semiconductor Alloys"

Ph.D., Dan Teng, 1990

Director: Kathie E. Newman
"Structural and Electronic Properties of Ordered Ternary III-V Semiconductors"

Other Students, Postdocs, and Visitors Advised

Ph.D. students

Madan Lamichhane, co-advised by J.D. Gezelter (current)

Masters students

Shan Huang, 2007
Xiaoou Xiang, 1990
Vandana Srivastava Chakravarti, 1985

REU students

Deanna A. Linn (a.k.a. Diana Gutierrez Zedano), University of Idaho, 2013
Jordan Hernandez, Tarleton State University, Texas, 2012
Nishanth Sasankan, University of Texas, Austin, 2011
Christina Gower, Loyola Marymount University, 2010
Dawn Fox, Southern Indiana University, 2009
Scott Gustafson, University of California, San Diego, 2008

Postdocs and Visitors

Hannah Fox, postdoc, co-advised by S.A. Corcelli and W.F. Schneider, 2008-2010
Richard J. Cohen, postdoc (1990-1993)
Jeffrey R. Gregg, postdoc (1987-1989)
Professor Bing-Lin Gu, visiting scholar, 1985-1987 (became President of Tsinghua University, Beijing)