

MARK EBERHART

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Colorado School of Mines
Golden, Colorado 80401

EDUCATION

B.S., University of Colorado, Applied Mathematics and Chemistry, 1977

M.S., University of Colorado, Physical Biochemistry, 1979

Ph.D., Massachusetts Institute of Technology, Materials Science and Engineering, 1983

PRESENT POSITION

Professor, Department of Chemistry and Geochemistry, Colorado School of Mines,
Golden, Colorado 80401

PROFESSIONAL EXPERIENCE

Head, Molecular Theory Group, 6/1993-present. This group coordinates and provides facilities for the computational components of materials research and education at Colorado School of Mines. Currently, the MTG maintains graphics and electronic structure software that is available to the CSM community as a whole.

Jefferson Science Fellow—Science Advisor to the Special Envoy for Energy Affairs, US Department of State, 9/2011-8/2012. Assisted in the development of energy related policies through technology assessment and scientific advice across the Bureau of Energy Resources (ENR). Developed communication strategies and acted as a liaison between ENR and the National Academies. Chaired the interagency ad hoc committee, *Narratives for Energy and Climate Change*, with representation from ENR, the Whitehouse Office of Science and Technology Policy, and ARAPA-E.

Research Associate Professor, Department of Metallurgical and Materials Engineering, Colorado School of Mines, Golden, Colorado, 1992-1998. Research focused on atomic scale interactions and their relationships to mechanical, catalytic, and transport properties of materials, with particular emphasis on the mechanical properties of metals and alloys. Directed graduate research focused on catalysis design, and various aspects of computational materials science aimed at modeling transport in ceramic and polymeric membranes.

Director, Laboratory for Materials Synthesis, Massachusetts Institute of Technology, Cambridge, Massachusetts, 1990-1992. Coordinated an interinstitutional program involving Harvard University, Imperial College, MIT, and Los Alamos National Laboratory in a program of computationally aided materials synthesis.

Staff Scientist, Los Alamos National Laboratory, Los Alamos, New Mexico, 1985-1990. Conducted research through the Materials Science and Technology Division in the modeling of environmental effects on mechanical properties of metals and alloys. Coordinated these modeling activities with alloy designers at Los Alamos, MIT and

Martin Marietta Research Labs in an attempt to improve high temperature intermetallic alloys. Supervised graduate research.

Research Associate, Materials Processing Center, Massachusetts Institute of Technology, Cambridge, Massachusetts, 1985-1990. Conducted research in corrosion and hydrogen embrittlement, supervised graduate student research.

Postdoctoral Research Associate, Department of Materials Science, Massachusetts Institute of Technology, Cambridge, Massachusetts, 1983-1985. Conducted research in application of electronic structure calculations toward an understanding of mechanical behavior. Supervised graduate student research.

VISITING APPOINTMENTS

Jefferson Science Fellow, United States Department of State, Bureau of Energy Resources, Science Adviser to the Special Envoy for Energy Affairs, 9/2011 – 8/2012

Visiting Scholar, Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois, 2004-2005

Visiting Scientist, Blackett Laboratory, Imperial College, London, UK, 1987 & 1991 to 1992

Visiting Scientist, Department of Chemistry, Harvard University, Cambridge, Massachusetts, 1990-1991

HONORS AND AWARDS

First Richard F. W. Bader Memorial Lecture, Exeter, UK, May 2012

Jefferson Science Fellow, 2011-2012

President, CSM Faculty Senate, August 2009-August 2010

CSM Favorite Instructor Award, October 2007

Member of the Board of Visitors, Army Research Office's Chemistry Division 2010-2012

Chair, Materials Reliability subgroup of the National Academy Panel on Materials Science and Engineering 2008-2010

Member of the National Academy Panel on Armor and Armaments 2007-2012

Member of the Board of Visitors, Army Research Office's Materials Science Division 2007-2009

Member of the National Research Council's planning committee for the workshop entitled "*Toward Sustainable Critical Infrastructure Systems: Framing the Challenges.*" March 2008

CSM Senior Class and Alumni Association Outstanding Faculty Award from the Department of Chemistry and Geochemistry, April 2006

American Chemical Society Diplomacy Fellow 2004-2005

Martin Marietta Research Excellence Grant 1988

TEACHING AND RELATED ACTIVITIES

COURSES TAUGHT

Computational Chemistry Field Session Module, CHGN 490
Introduction to Solid State Chemistry, CHGN 198
Materials Structure and Bonding, MLGN 593
Computational Chemistry, CHGN 475
Physical Chemistry I & II, CHGN 351 & 353
Materials Systems, SYGN 202
Materials Bonding, ML 513
Processing/Structure/Property/Performance Relations in Materials Design, MLGN 590
Perspectives in Materials Science, ML 591
Freshman Success Seminar, CSM 101
Freshman Chemistry I & II, CHGN 121 & 124/122
Technology and Society, HNRS 300
Undergraduate Research, CHGN 495A
Advanced Physical Chemistry, CHGN 503
Chemical Thermodynamics Laboratory, CHGN 201
Engineering Thermodynamics, DC 209
Introduction to Biochemistry, CHGN428
Mechanics of Materials, EGGN320
Structure of Materials, MLGN 501
Advanced Topics in the Physics and Chemistry of Materials, CHGN 504
Engineering Practices I & III, undergraduate
Introduction to Physical Chemistry-Thermodynamics (no longer offered)
Quantum Chemistry, undergraduate (no longer offered)

COURSE DEVELOPMENT

Developed Physical Chemistry Field Session Module
Developed Introduction to Solid State Chemistry—Currently offered as CHGN 198
Developed Computational Chemistry, CHGN 475
Co-developed Physical Chemistry I and II, CHGN 351 and 353
Co-developed DC 209
Developed (restructured) Materials Bonding ML 513

ADVISING

Post Doctoral Advising

Travis Jones, Topological and Geometric Structure of the Chemical Bond, Postdoctoral Fellow Colorado School of Mines, 2011-2012

Shannon Willoughby, Modeling Magnetic Materials, Postdoctoral Fellow Colorado School of Mines, 2003-2004

Adam Stern, Tools for Charge Density Analysis, Postdoctoral Fellow CSM and Tulane University, 2003

James MacLaren, Development and Application of the LKKR Method, Director Funded Post Doc, Los Alamos National Laboratory, 1987-1999

Michael McHenry, Modeling and Theory of Magnetism and Superconductivity, Director Funded Post Doc, Los Alamos National Laboratory, 1999

Michele Donovan, Modeling Metal Ceramic Interfaces, Visiting Post Doc, MIT & Los Alamos National Laboratory, 1999-2000

Dennis Clougherty, Density Functional Theory, Visiting Post Doc, MIT & Los Alamos National Laboratory, 1999

Ph. D. Students

Tim Wilson, Chemistry and Geochemistry*, Colorado School of Mines, current, *Bondalyzer with Applications to Molecular and Solid State Phenomena*

Erica Lotspeich, Chemistry and Geochemistry*, Colorado School of Mines, current, *Atom Probe Tomographic Studies of Explosives*

Michael Hoerner, Co-advisor with John Speer-Metallurgical and Materials Engineering, Colorado School of Mines, current, *First principles Investigations of Grain Boundary Mobility in Austenite*

Amanda Morgenstern, Chemistry and Geochemistry, Colorado School of Mines, current, *Conceptual Density Functional Theory in Enzyme Design*

Jonathan Miorelli, Chemistry and Geochemistry, Colorado School of Mines, current, *Advancing Conceptual Density Functional Theory*

Travis Jones, Chemistry and Geochemistry, Colorado School of Mines, 2011, *The Irreducible Bundle: Its Method, Content, and Meaning*

Robert Torget, co-advisor, Chemistry, Colorado School of Mines
Theory Assisted Design of Photolytic Materials

Wongasa Kritiporn, Materials Science, Colorado School of Mines,
Aesthetics and the Extension of Ashby Diagrams

Mike Jacobs, co-advisor, Chemistry, Colorado School of Mines, 2008,
Experimental and Theoretical Investigation of Au-CN complexes on Gold Surfaces

Scott Plummer, co-advisor, Ph. D. Chemistry, Colorado School of Mines, 2007,
Photosynthetic hydrogen Production from Green Alga Chlamydomonas Reinhardtii

Tomoko Kito, co-advisor, Ph. D. Materials Science, Colorado School of Mines, 1996,
The Evaluation and Characterization of Acid Catalysts Used in An On-Board Diethyl Ether Generator for Cold Start Assistance of an Ethanol-Fueled Vehicle

Michele Donovan, co-advisor, Ph. D. Materials Science and Engineering, MIT, 1989,
A Theoretical Investigation of Electronic Structure and Auger Transitions in Iron, Copper and Their Oxides

Michael McHenry, co-advisor, Ph. D. Materials Science and Engineering, MIT, 1988,
Electronic Structure and Magnetism in Metallic Alloys Exhibiting Local Icosahedral Order

Simon Crampin, co-advisor, Ph. D. Physics, Imperial College, 1988,
Self-Consistent Charge Densities at Isolated Planar Defects in Metals

M.S. Students

Matt Sauer, co-advisor, Materials Science Program, Colorado School of Mines, 2010,
Quench and Partitioning of Transition Carbides Stability

Travis Jones, Chemistry and Geochemistry, Colorado School of Mines, 2010
The Theory and Application of Special Gradient Paths to Chemistry and Materials

Wongasa Kritiporn, M.S. (non-thesis), Colorado School of Mines, 2006

Helen Kearney, co-advisor, M.S. Materials Science, Colorado School of Mines, 2005,
Characterization of Trace Elements in a Petrified Wood Material for Provenience Studies

Janine Rowsey, M.S. Materials Science, Colorado School of Mines, 2001,
Feasibility of Sourcing Petrified Wood artifacts in the Denver Basin and Adjacent Foothills

Erika Knoerr, M.S. Chemistry, Colorado School of Mines, December 2000,
Charge Density Based Reactivity Model for an SN2 Reaction

Undergraduates Research

Tim Wilson, B.S. Chemical and Biological Engineering CSM (5-2014), to continue at CSM as graduate student fall 2014.

Travis Jones, B.S. Chemistry CSM, subsequently began graduate studies at CSM Chemistry

Ken Light, B.S, Chemistry and Chemical Engineering CSM, subsequently began graduate studies at Stanford University

Yeong-Do Park, B.S. Metallurgical Engineering CSM, subsequently began graduate studies at Cal Tech

SPONSORED RESEARCH (since 2001)

Office of Naval Research, The Discovery and Application of Charge Density Property Relationships, 6/1/14 to 5/31/17, PI, \$330,000.

Office of Naval Research, Theoretical Investigation of Amorphous Metals, 3/1/10 to 2/28/13. PI, \$330,000.

Army Research Office, Charge Density Engineering: A Feasibility Study, 9/1/10 to 8/31/13, Co-PI, \$360,000

Clean Coal Technology, 6/1/08 to 5/31/10, Co-PI, \$1,000,000.

Water Reuse Foundation, *Predictive Models to Aid in Design of Membrane Systems for Organic Micropollutants Removal*, 11/1/2007 to 4/30/2010, Co-PI with Jörg Drewes (ESE), \$467,000

Office of Naval Research, *Design Research Tools*, Renewal, 7/1/08 to 6/23/10, PI, \$150,000.00

Defense Advanced Research Projects Administration, *Design of Amorphous Materials*, 9/1/06 to 8/31/08, PI, \$166,000.00

Office of Naval Research, *Design Research Tools*, 6/27/05 to 6/30/2008, PI, \$225,000

Questek, *Iron based metallic glasses*, 10/1/03 to 9/30/04, PI, \$25,000.00

Colorado State Historical Fund Grant, *Analysis of Petrified Wood Artifacts*, Co-PI with Craig Simmons, 9/1/2003 to 8/31/2006 \$119,234.00

Defense Advanced Research Projects Administration, *Theory Assisted Materials Design*, 9/1/01 to 8/31/04, PI, \$450,000.00

Air Force Office of Scientific Research Subcontract through Northwestern, *Design of High Temperature Nb Alloys*, 10/1/01 to 9/30/04, PI, \$225,000.00

Colorado Advanced Materials Institute, *Sourcing Lithic Materials*, 10/1/01 to 6/30/02, PI \$31,000.00

PUBLICATIONS

BOOKS, ARTICLES, REPORTS

“Sustainable Critical Infrastructure Systems: A Framework for Meeting 21st Century Imperatives,” National Research Council Report

“Why Things Break: Understanding the world by the way it comes apart,” Harmony Books, 2003.

“Feeding the Fire: The lost history and uncertain future of mankind’s energy addiction,” Harmony Books, May 2007

“Energy and the Curse of Interesting Times,” *Mines: Colorado School of Mines Magazine*, Spring/Summer 2007

“Going to Extremes: Materials Science and Engineering,” *Mines: Colorado School of Mines Magazine*, Spring/Summer 2007

“Why Things Break,” M.E. Eberhart, *Scientific American*, February 1999.

REFEREED PUBLICATIONS

- 86) “An Electronic Criteria for Assessing Intrinsic Brittleness of Metallic Glasses” T.E. Jones, X.F. Wang, Y. Wu, Z. Lu, S. Halas, T. Durakiewicz, and M.E. Eberhart, Journal of Chemical Physics, **141**, 024503 (2014).
- 85) “Reactive Cluster Model of Metallic Glasses,” T.E. Jones, M.E. Eberhart, Journal of Chemical Physics, **140**, 84501 (2014).
- 84) “The Two Faces of Chemistry: Can they be reconciled?,” M.E. Eberhart, and T.E. Jones, Foundations of Chemistry, **15**, 1-9, (2012).
- 83) “Cauchy Pressure and the Generalized Bonding Model for Nonmagnetic BCC Transition Metals” M.E. Eberhart, and T.E. Jones, Physical Review B, **86**, 134106, (2012).
- 82) “Better Alloys with Quantum Design,” T.E. Jones, M.E. Eberhart, S. Imally, C. Mackey, and G.B. Olson, Physical Review Letters, **109**, 125506, (2012).
- 81) “A Surface Enhanced Raman Spectroscopy and Density Functional Theory Study of Au[CN]₂⁻/Au[CN]₄⁻ Adsorbed on Gold Nanoparticles,” M.B. Jacobs, T.E. Jones, M.E. Eberhart, and P.W. Jagodzinski, Journal of Phys. Chem. C, **115**, 24115-24122, (2011).
- 80) “Bond bundles and the Origin of Functionality,” T.E. Jones, M.E. Eberhart, S. Imally, and C. Mackey, Journal of Phys. Chem. A, **115**, 12582, 2011 (invited).
- 79) “Topological Catastrophe and Isostructural Phase Transition in Calcium.” T.E. Jones, M.E. Eberhart, and D.P. Clougherty, Physical Review Letters, **105**, 265702 (2010).
- 78) “Topology of the Charge Density in Ru and Zr,” T.E. Jones and M.E. Eberhart, ACTA Crystal A. **65**, 141-144, 2009.
- 77) “The Bond Bundle in Open Systems,” T.E. Jones and M.E. Eberhart, International Journal of Quantum Chemistry, **110**, 1500–1505 (2010).
- 76) “The Irreducible Bundle: Further Structure in the Kinetic Energy Distribution”, T.E. Jones, and M.E. Eberhart, Journal of Chemical Physics, **130**, 204108 2009
- 75) “First Principles Study of Mode I Fracture of Fe/TiX Interfaces (X = C, N)”, T.E. Jones, M. Sauer, and M.E. Eberhart, Physical Review B, **78**, 092104 2008.
- 74) “Topology of the Spin-polarized Charge Density in bcc and fcc Iron”, T.E. Jones, M.E. Jones, and D.P. Clougherty, Physical Review Letters, **100**, 017208, 2008.
- 73) “A Jahn-Teller Model for Metallic Glass Structure and Stability,” M.E. Eberhart, T.E. Jones, D.P. Clougherty.
- 72) “Electronic Selection Rules Controlling Dislocation Glide in BCC Metals” T.E. Jones, M.E. Eberhart, D.P. Clougherty and C. Woodward, Physical Review Letters, **101**, 085505, 2008
- 71) “Visualizing the Metallic Bond,” M.E. Eberhart, T.E. Jones, and M. Sauer, Journal of Metals, **60**, 67-72, 2008.
- 70) “Molecular Orbital Model for Pyridine/a-Pyridyl Adsorption on Metal Surfaces,” T.E. Jones, M.E. Eberhart, C. Zuo, and P.W. Jagodzinski, J. Phys. Chem. C, **111**, 5493 (2007)

- 69) "Theory and Application of Dissociative Electron Capture in Molecular Identification" C.D. Havey, M.E. Eberhart, T.E. Jones, K.J. Voorhees, J.A. Laramée, R.B. Cody, and D.P. Clougherty, *J. Phys. Chem. A*, **110**, 4413 (2006)
- 68) "Structure Property Relationships in the Design of Alloy Composition: Moving Beyond Electron to Atom Ratios," M.E. Eberhart, T.E. Jones, M.A. Batchelder, and G.B. Olson, *J. Mater. Res.*, **20**, 1330 (2005)
- 67) "Looking for Design in Materials Design," M.E. Eberhart and D.P. Clougherty, (invited commentary), *Nat. Mater.*, **3**, 659 (2004)
- 66) "Quest for Noburnium: 1300C Cyberalloy," G.B. Olson, A.J. Freeman, P.W. Voorhees, G. Ghosh, J. Perepezko, M. Eberhart, and C. Woodward, *International Symposium on Niobium for High Temperature Applications*, Eds. Y-W. Kim and T. Carneiro (TMS, Warrendale, PA) 113 (2004)
- 65) "Quantum Mechanics and Molecular Design in the 21st Century," M.E. Eberhart, *Found. Chem.*, **4**, 201 (2002)
- 64) "Topology of Electronic Charge Density and Energetics of Planar Faults in fcc Metals," N. Kioussis, M. Herbranson, E. Collins, and M.E. Eberhart, *Phys. Rev. Lett.*, **88**, 3 (2002)
- 63) "Hydrogen Trapping in Ferritic Steel Weld Metal," I. Maroef, D.L. Olson, M. Eberhart, and G.R. Edwards, (invited), *Int. Mater. Rev.*, **47**, 191 (2002)
- 62) "Analysis of Nitrated Polycyclic Aromatic Hydrocarbons Using Electron Monochromator Mass Spectroscopy," K. J. Voorhees, R.B. Cody, M.E. Eberhart, and R. McCormick, *Proc. 49th ASMS Conference on Mass Spectrometry and Allied Topics* (2001)
- 61) "Charge Density-Shear Moduli Relationships in Aluminum-Lithium Alloys," M.E. Eberhart, *Phys. Rev. Lett.*, **87**, 205503 (2001)
- 60) "A Quantum Description of the Chemical Bond," M.E. Eberhart, *Philos. Mag. B*, **81**, 721 (2001)
- 59) "Silver Doped Nafion-poly(pyrrole) Membranes for Facilitated Permeation of Liquid-Phase Olefins," A. Sungpet, J.D. Way, C.A. Koval, and M.E. Eberhart, *J. Membr. Sci.*, **4905**, 1 (2001)
- 58) "Electron Density Based Representation of Reactivity for an S_N2 Reaction," E.H. Knoerr and M.E. Eberhart, *J. Phys. Chem.*, **105**, 880 (2001)
- 57) "Why Things Break," M.E. Eberhart, *Sci. Amer.*, **281**, 66 (1999)
- 56) "The Charge Redistribution Accompanying Slip and Cleavage: Electronic Structure Calculations in Alloy Design," M.E. Eberhart, C. Woodward, and A.F. Giamei, (invited) *MRS Symposium Proceeding*, **539**, 13 (1999)
- 55) "The Visualization and Use of Electronic Structure for Metallurgical Applications," M.E. Eberhart and A. Giamei, *Mater. Sci. Eng.*, **A248**, 287 (1998)
- 54) "From Topology to Geometry," M.E. Eberhart, (invited), *Can. J. Chem.*, **74**, 1229 (1996)

- 53) "A Chemical Approach to Ductile Versus Brittle Phenomena," M.E. Eberhart, *Philos. Mag. A*, **73**, 47 (1996)
- 52) "The Metallic Bond: Elastic Properties," M.E. Eberhart, *Acta Mater.*, **44**, 2495 (1996)
- 51) "Chemisorption of Small Molecules on Palladium in Terms of Local Density Functional Calculations", T. Kito and M.E. Eberhart, *Surf. Sci.*, **357-358**, 609 (1996)
- 50) "Van der-Waals Bonds," M.E. Eberhart, (invited), *Macmillan Encyclopedia of Physics*, Macmillan Press, (1996)
- 49) "Covalent Bonds," M.E. Eberhart, (invited), *Macmillan Encyclopedia of Physics*, Macmillan Press, (1996)
- 48) "The Origins of the Similarities Between Late Transition Metals and Early Transition Metal Monocarbides," M.E. Eberhart and J.M. MacLaren, (invited), *Proceedings of the 1995 International Chemical Congress of the Pacific Basin Societies*, Honolulu, Hawaii (1995)
- 47) "Computational Metallurgy," M.E. Eberhart, *Science*, **265**, 332 (1994)
- 46) "A Theoretical Investigation of the Mechanisms of Fracture in Metals and Alloys," M.E. Eberhart, J. MacLaren, and D.P. Clougherty, *J. Amer. Chem. Soc.*, **115**, 5762 (1993)
- 45) "Charge Density Topology and its Relationship to Properties in Intermetallic Alloys," M.E. Eberhart, J. MacLaren, and D.P. Clougherty, *Philos. Mag. B*, **68**, 455 (1993)
- 44) "Bonding-Property Relationships in Intermetallic Alloys," M.E. Eberhart, J.M. MacLaren, and D.P. Clougherty, *J. Mater. Res.*, **8**, 438 (1993)
- 43) "Ab initio Investigations of Oxygen Diffusion in Group IB Transition Metals," M.E. Eberhart, M.M. Donovan, and R.A. Outlaw, *Phys. Rev.*, (1992)
- 42) "Interface Electronic and Magnetic Structures of Layered Fe in Contact with MgO," Y.K. Kim, M.E. McHenry, M.P. Oliveria, and M.E. Eberhart, *Mat. Res. Soc. Symp. Proc.*, **238**, 799 (1992)
- 41) "Towards a Chemistry of Cohesion and Adhesion," M.E. Eberhart, M.M. Donovan, J. MacLaren, and D.P. Clougherty, (invited), *Prog. Surf. Sci.*, **36**, 1 (1991)
- 40) "Geometrical Origins of Interfacial Strength," M.E. Eberhart, D.P. Clougherty, and J.N. Louwen, (invited), *MRS Bull.*, **16**, 53 (1991)
- 39) "Bonding and Electronic Structure of Nb/C and Nb/NbSi₂ Interfaces," M.M. Donovan, J.M. MacLaren, M.E. Eberhart, and A.R. Barron, *Mat. Res. Soc. Symp. Proc.*, (1991)
- 38) "Magnetic and Electronic Properties of Au/Fe Superlattices and Interfaces," J.M. MacLaren, M.E. McHenry, M.E. Eberhart, and S. Crampin, *J. Appl. Phys.*, **67**, 5406 (1990)

- 37) "Interface Electronic Structure of XDTM Titanium Aluminide Composites," D.D. Vvedensky, M.E. Eberhart, L. Christodoulou, S. Crampin, and J.M. MacLaren, Mater. Sci. Eng., **A126**, 33 (1990)
- 36) "An Electronic Model for the DO₂₂ to L₁₂ Transformation of the Group IV-A Trialuminides" M.E. Eberhart, K.S. Kumar, and J.M. MacLaren, Philos. Mag., **61**, 943 (1990)
- 35) "Mechanisms for Cleavage and Intergranular Embrittlement in Fe," M.E. Eberhart and J.M. MacLaren, (invited), *Sagamore Army Material Research Conference*, **34**, 693 (1990)
- 34) "Quantum Mechanics and Mechanical Properties: Towards 21st--Century Materials," M.E. Eberhart, S. Crampin, J.M. MacLaren, and D.D. Vvedensky, Contemp. Phys., **31**, 73 (1990)
- 32) "Bonds, the Transition State and Fracture," M.E. Eberhart, J.M. MacLaren, M.E. McHenry, and S. Crampin, *Acta-Scripta. Met.*, (Proceedings Series), **4**, 71 (1990)
- 31) "Electronic Structure of Extended Defects in Close Packed Metals," S. Crampin, D.D. Vvedensky, M.E. Eberhart, and J.M. MacLaren, *Mat. Res. Soc. Symp. Proc.*, **141**, 373 (1989)
- 30) "Electronic Structure Near a (210) Tilt Boundary in Nickel," S. Crampin, D.D. Vvedensky, J.M. MacLaren, and M.E. Eberhart, Phys. Rev. B, **40**, 3413 (1989)
- 29) "Mechanical Stability and Charge Densities at Stacking Faults," J.M. MacLaren, S. Crampin, D.D. Vvedensky, and M.E. Eberhart, Phys. Rev. Lett., **63**, 2586 (1989)
- 28) "Local Moment Formation on Fe in Alkali Metal Hosts," M.E. McHenry, J.M. MacLaren, D.D. Vvedensky, and M.E. Eberhart, Phys. Rev. B., **40**, 10111 (1989)
- 27) "Grain Boundary Electronic Structure and Materials Design," M.E. Eberhart and D.D. Vvedensky, in *Grain Boundary Chemistry and Intergranular Fracture*, G. Was ed., (1988)
- 26) "Symmetry-Induced Local Magnetic Moments in Icosahedral Al-Mn Alloys," M.E. McHenry, D.D. Vvedensky, M.E. Eberhart, and R.C. O'Handley, Phys. Rev. B, **37**, 10887 (1988)
- 25) "Model for Ductility Enhancement in L₁₂ Intermetallic Compounds," M.E. Eberhart and D.D. Vvedensky, Scr. Metall., **22**, 1183 (1988)
- 24) "Environmentally Specific Mechanical Properties: Beyond Atomic Parameters" M.E. Eberhart and D.D. Vvedensky, Phys. Rev. B, **37**, 8488 (1988)
- 23) "Bond Strain at Grain Boundaries," M.E. Eberhart and D.D. Vvedensky, Phys. Rev. Lett., **59**, 1981 (1988)
- 22) "Toward a Microscopic Basis of Mechanical Behavior," D.D. Vvedensky and M.E. Eberhart, Philos. Mag. Lett., **55**, 157 (1987)
- 21) "Localized Grain Boundary Electronic States and Intergranular Fracture," M.E. Eberhart and D.D. Vvedensky, Phys. Rev. Lett., **58**, 61 (1987)

- 20) "Theoretical Approaches to Materials Design: Intergranular Embrittlement," D.D. Vvedensky and M.E. Eberhart, (invited) *Proceedings of the NATO Advanced Research Workshop on the Chemistry and Physics of Fracture*, Eds., R.M. Latanision and R.H. Jones, Plenum Press, NY, 163 (1987)
- 19) "Local Atomic Order and Magnetic Properties of Non-crystalline Alloys," R.C. O'Handley, M.E. Eberhart, and N.J. Grant, in *Amorphous Metals and Semi-Conductors*, Eds., P. Hasen and R.I. Jaffee, Pergamon Press, NY, 241 (1986)
- 18) "Calculated Electronic Structure of Icosahedral Al and Al-Mn Alloys," M.E. McHenry, M.E. Eberhart, R.C. O'Handley, and K.H. Johnson, *Phys. Rev. Lett.*, **56**, 81 (1986)
- 17) "Molecular Orbital Models of Melting and the Amorphous State," M.E. Eberhart, K.H. Johnson, D. Adler, and R.C. O'Handley, *J. Non-Cryst. Solids*, **83**, 12 (1986)
- 16) "The Effects of Bond Bending in Silane," M. Milner, M.E. Eberhart, D. Adler, and K.H. Johnson, *J. Chem. Phys.*, (1986)
- 15) "The Electrochemistry and Solid-State Chemistry of Intergranular Hydrogen Embrittlement," M.E. Eberhart and R.M. Latanision, (invited), *Modeling Environmental Effects*, Ed., R. Jones, The Metallurgical Society of AIME, Plenum (1986)
- 14) "Quantum Mechanics and Fracture," M.E. Eberhart, (invited), *Advances in the Mechanics and Physics of Surfaces*, **3** (invited), Eds., R.M. Latanision and T.E. Fischer, Harwood Academic Publishers (1986)
- 13) "The Chemistry of Fracture - A Basis for Analysis," M.E. Eberhart, R.M. Latanision, and K.H. Johnson, *Acta Metall.*, **33**, 1769 (1985)
- 12) "Molecular Orbital Models for the α - γ Transformation of Cerium," M.E. Eberhart, *Solid State Comm.*, **54**, 187 (1985)
- 11) "Theoretical Studies of Aromatic Silicon-Based Structures and Their Application to Photostructural Changes in Hydrogenated Amorphous Silicon," S.A. Zygmunt, M.E. Eberhart, K.H. Johnson, and D. Adler, *J. Non-Cryst. Solids*, **75**, 297 (1985)
- 10) "The Jahn-Teller Effect and Icosahedral Stability in Metallic Glasses," M.E. Eberhart, K.H. Johnson, D. Adler, R.C. O'Handley, and M.E. McHenry, *J. Non-Cryst. Solids*, **75**, 97 (1985)
- 9) "Molecular Orbital Models for Structural Phase Transformations in Crystalline and Amorphous Cobalt Alloys," M.E. Eberhart, K.H. Johnson, and R.C. O'Handley, *Phys. Rev. B*, **29**, 1097 (1984)
- 8) "EPR Parameters of Quantum Mixed-Spin Ferric Complexes with Rhombic and Tetragonal Symmetry," M.M. Maltempo and M.E. Eberhart, *Chem. Phys. Lett.*, **108**, 204 (1984)
- 7) "A Molecular Orbital Model of Intergranular Embrittlement," M.E. Eberhart, K.H. Johnson, and R.M. Latanision, *Acta Metall.*, **32**, 955 (1984)

- 6) "Metastable Defects in Amorphous Silicon Alloys," D. Adler, M.E. Eberhart, K.H. Johnson, and S.A. Zygmunt, *J. Non-Cryst. Solids*, **66**, 273 (1984)
- 5) "Electronic Structure of Metallic Glasses," M.E. Eberhart, F.A. Leon, and K.H. Johnson, *Chemistry and Physics of Rapidly Solidified Materials*, (invited), Eds., B.J. Berkowitz and R.O. Scattergood, The Metallurgical Society of AIME, 139 (1983)
- 4) "Molecular Orbital Models of Melting and Glass Formation," M.E. Eberhart, K.H. Johnson, and R.C. O'Handley, *Rapidly Solidified Amorphous and Crystalline Alloys*, Eds., B.H. Kear and B.C. Giessen, North-Holland, N.Y., 103 (1982)
- 3) "Theoretical Models for the Electronic Structure of Hydrogenated Amorphous Silicon II: Three Center Bonds," M.E. Eberhart, K.H. Johnson, and D. Adler, *Phys. Rev. B*, **26**, 3138 (1982)
- 2) "Resistivity of Amorphous Co-Mn-B Alloys, Beyond the s-d Model," M.E. Eberhart, K.H. Johnson, and N.J. Grant, *J. Appl. Phys.*, **53**, 8321(1982)
- 1) "Molecular Orbitals and the Atomistics of Fracture," M.E. Eberhart, K.H. Johnson, R.P. Messmer, and C.L. Briant, (invited), *Proceedings Atomistics of Fracture*, May 21-31, 1981, Eds., R.M. Latanision and J.R. Pickens, Plenum Press, NY.

BOOK REVIEWS

I am asked to review books on a regular basis. I accept these offers as time permits. Two recent reviews are for *Vanity, Vitality, and Virility: The Science Behind the Products You Love to Buy*, by John Emsley; and *Euler's Formula*, by Paul Nahan

PATENTS AND APPLICATIONS

"The bond bundle in open system," through CSM and licensed by TecPlot (Seattle WA.) 2007

"Prediction of electron capture resonance spectroscopy," through University of Vermont, 2006

PRESENTATIONS

MAJOR AND PLENARY LECTURES (2002–2014)

"Beyond the Ball and Stick," *International Conference on Chemical Bonding*, Kauai, HI July 24-28, 2014

"Design with the Quantum Theory of Atoms in Molecules" Richard Bader Memorial Lecture, First World Congress on MIRCE Mechanics, Exeter, UK, May 28, 2012

"Science, Energy, and the National Strategic Narrative," Jefferson Science Fellow Lecture, US Department of State Marshall Auditorium, January 31, 2012

"How Things Break," *Spontaneous Energy Focusing Phenomena and Multiscale Physics*, Singapore, Singapore, August 30-September 3, 2010

"The Bond and Bond Bundle in Materials Design," *Eleventh International Conference on Advanced Materials*, Rio de Janeiro, September 16-20 2009

“Materials Design: Lessons from Synthetic Organic Chemistry,” *Eighteenth International Materials Research Congress 2009*, Cancún, Mexico, August 16-21 2009

“Charge Density Descriptors,” *First International Conference on Materials Informatics and DFT*, Oran, Algeria, October 12-15 2008

“Bonds in Molecules,” *Fifth European Charge Density Conference*, Lake Como, Italy June 6-11, 2008

“Mining First Principle Cluster Calculations for Alloy Design,” *Materials Design Workshop*, Bangalore, India, October 29-November 2, 2007

“The Hammond Postulate and Materials Design,” *Third International Workshop on DFT Applied to Metals and Alloys Incorporating the Materials Genome Project* Oran, Algeria, May 2-4, 2007

“The Slowly Evolving Picture of Electronic Structure: The Curse of Quantum Mechanics and Digital Computers,” *Workshop on Engineering Theory: Science in the Context of Application*, Center for Interdisciplinary Research (ZiF), Bielefeld, Germany, May 2-3, 2007

“The Inverse Problem: A rose by another name,” *The Fourth International Conference on Materials Design*, Tlemcen, Algeria, May 1-4, 2006

“Quantum Mechanics and the Design of Amorphous Alloys,” *DARPA program on Structural Amorphous Metals*, Santa Fe, New Mexico, March 31-April 2, 2003

INVITED LECTURES (2002–2014)

“Bond Bundles: Toward an Understanding of Solid State Transformations,” ACS Fall Meeting, August 10-14, 2014, San Francisco, symposium on Mechanisms, Kinetics, and Thermodynamics of Solid State Transformations: Experiment and Theory

“Schrödinger’s Microscope,” *SRG*, Evanston, Illinois, March 25-26, 2013

“Structure in Structure in Structure” *International School for Advanced Studies*, Trieste, Italy, September 19, 2012

“Theoretical Investigations of the Structure and Properties of Metallic Glasses” *ONR Research Highlights*, Arlington VA. 11 October 2011

“Charge Density Analysis for Interfacial Strength,” *SRG-25*, Evanston, Illinois, March 21-22, 2011

“Topological Properties of the Charge Density and Fracture,” *SRG-24*, Evanston, Illinois, March 22-23, 2010

“Further Developments in the Topological Analysis of the 3D Charge Density,” *Design Research Tools Annual Review*, Arlington VA, July 13-15, 2010

“*Ab initio* Methods in Materials Design,” MRL Wright-Patterson AFB, 13 August, 2010

“*Ab initio* Methods in Materials Design,” ARL Aberdeen, MD, 20 September 2010

“The Writing of *Why Things Break*,” Jefferson County Historical Society, Mount Vernon Country Club, 4 October 2008.

“Further Developments in the Topological Analysis of the 3D Charge Density,” *Design Research Tools Annual Review*, Columbus Ohio, August 8-11, 2008

“Topological properties of the Charge Density and Fracture,” *SRG-23*, Evanston, Illinois, March 24-26, 2008

“Developments in the Topological Analysis of the 3D Charge Density,” *Design Research Tools Annual Review*, Evanston, Illinois, August 21-24, 2007

“Linking Science and Policy,” *National Conference of State Legislatures—Energy Policy Session*, Boston, Massachusetts, August 7-10, 2007

“Feeding the Fire,” *Boulder Book Store*, Boulder, Colorado, 23 May 2007

“Feeding the Fire,” *Tattered Cover*, Highland Ranch, Colorado, 22 May 2007

“Charge Density Topology,” *SRG-22*, Evanston, Illinois, March 19-21, 2007

“Computer Graphic and First Principle Methods: An Opportunity,” *Techplot*, Seattle, Washington, 7 December 2006

“The Past, Present, and Future of the Chemical Bond,” *Department Colloquium*, *University of Colorado*, Colorado Springs, Colorado, 31 October 2006

“Feeding the Fire: Planning an energy future,” *Colorado Café Scientifique*, Denver, Colorado, 19 September 2006

“Metallic Glass Structure and Stability: A basis for quantum design,” *DARPA Kickoff Meeting for Structural Amorphous Materials II*, Washington D.C., 17 August 2006

“The Chemical Bond in 3D,” *ONR D3D Consortia Meeting*, Arlington, Virginia, June 12-14, 2006

“Charge Density Topology,” *SRG-2006*, Evanston, Illinois, March 22-23, 2006

“The Inverse Problem,” *Colloquium, Department of Materials Science*, McMaster University, Hamilton, Ontario, 21 March 2006

“What I Did Last Year,” *Sabbatical Presentation to the CSM Board of Trustees*, Golden, Colorado, 27 January 2006

“Why Things Break,” *CSM Alumni Association*, Denver, Colorado, 6 December 2005

“Three Dimensional Bonding at Interfaces,” *ONR D3D Consortia*, Ohio State University, Columbus, Ohio, October 17-19, 2005

“Bond Analysis Tool,” *D3D Kickoff Meeting*, Arlington, Virginia, 29 April 2005

“Metallic Glass Structure and Stability: A basis for quantum design,” *CSM Materials Research Seminar*, Golden, Colorado, 6 October 2005

“Electronic Basis for Glass Stability,” *Steel Research Group*, Evanston, Illinois, March 21-23, 2005

“Noburnium: Oxygen solubility,” *Questek*, Evanston, Illinois, 15 July 2004

“Noburnium: Oxygen diffusion and solubility,” *The Twentieth Annual Meeting of the Steel Research Group*, Northwestern University, Evanston, Illinois, March 22-24, 2004

“Picostructure-Property Relationships,” *The Nineteenth Annual Meeting of the Steel Research Group*, Northwestern University, Evanston, Illinois, March 17-19, 2003

“Quantum Mechanics in Materials Design.” *Materials Directorate, Wright Patterson Air Force Base*, Dayton, Ohio, 30 August 2002

“Materials Design Approaches,” *Materials Directorate, Wright Patterson Air Force Base*, Dayton, Ohio, 9 May 2002

OTHER SIGNIFICANT INVITED LECTURES

“The Charge Redistribution Accompanying Slip and Cleavage: Electronic Structure Calculations in Alloy Design,” *MRS Fall Meeting*, Boston, Massachusetts, November 30 - December 4, 1998

“The Chemical Bond: Elastic Properties” *MIT Materials Science Colloquium*, Cambridge, Massachusetts, 20 January 1997

“The Chemical Bond and Fracture,” *ASM-TMS*, Chicago, Illinois, 19 November 1996

“The Origins of the Similarities Between Late Transition Metals and Early Transition Metal Monocarbides,” *The 1995 International Chemical Congress of the Pacific Basin Societies*, Honolulu, Hawaii, December 17-22, 1995

“The Chemistry of Hydrogen Embrittlement,” *Hydrogen in Naval Structures*, Defense Strategic Technology Organization, Melbourne, Australia, October 1996

“Toward Twenty First Century Materials,” *Physical Metallurgy Gordon Conference on Materials Design*, Plymouth State College, Plymouth, New Hampshire, August 1-6, 1993

“Chemical Mechanism of Hydrogen Embrittlement.” *NATO Advanced Study Institute on Hydrogen Embrittlement*, Munich, F.R. Germany, June 19-23, 1989

“The Chemistry of Fracture,” *National Research Council, Materials Advisory Board*, Washington DC, February 1988

“Mechanisms for Cleavage and Intergranular Embrittlement in Fe,” *Sagamore Army Material Research Conference*, Lake George, New York. August 30 - September 3, 1987

“Computational Methods in Alloy Design”, *National Research Council, Materials Advisory Board, Workshop*, La Jolla, California, March 1987

“Quantum Mechanics and Fracture”, *Physical Metallurgy Gordon Conference*, Tilton School, Tilton, New Hampshire, July 28 - August 2, 1987

“Theoretical Approaches to Materials Design: Intergranular Embrittlement,” *NATO Advanced Research Workshop on the Chemistry and Physics of Fracture*, Bad Reichenhall, F.R. Germany, 22 June 1986

“Molecular Orbital Models of Embrittlement Phenomena” *International Conference on Fundamentals of Fracture*, Gatlinburg, Maryland, June 1986

“Molecular Orbital Models of Fracture,” *Bernd Matthias Lecture*, Los Alamos, New Mexico, April 1985

INTERVIEWS – APPEARANCES

Television

NOVA, “Making Stuff Stronger” in the “Making Stuff” series, first aired 2011.

International

BBC, The Material World, 10/2003

National

USA Radio Network, Daybreak USA

ABC Radio, Morning Show

KPOJ-AM, Thom Hartman Show

Coast to Coast with George Noory

Local Radio

Hartford/New Haven, WXML-FM, Morning Show

Hartford, WPLR-FM, Morning News

Philadelphia, KYW-AM New Features

Baltimore/Ocean City, WOCM-FM, Morning Show

Indianapolis, Metro-Networks, News Features

Indianapolis, WHBU-AM, Morning Show

Green Bay, WEON-AM, Morning Show

Rochester, WHAM-AM, Morning Show

Pittsburgh, WMKX-FM/WJNG-FM, Morning Show

San Jose, KKUP-FM, Morning Show

Pennsylvania and Ohio, WOHI-AM, Midday Show

Milwaukee, WRJN-AM, News Makers

Seattle, KPTK-AM, Community Matters

Connecticut, New York, and New Jersey, WICC-AM, Davis Smith’s Exchange

Kansas City, KCTE-AM, Live with Jay

Cleveland, WMJI, Lanigan & Malone

Pittsburgh, KDKA, Mike Pinetek Show

Burlington, IA, KCPS-AM, Morning Show

San Francisco, KVON, Morning Edition

Marin County, CA, KWMR, Wake Up Marin

PROFESSIONAL SOCIETIES

American Chemical Society

Materials Research Society

PROFESSIONAL SERVICE

Chair-elect (2005), Local Section American Chemical Society

Chair (2006), Local Section American Chemical Society

REVIEWS

I review ten to fifteen journal submissions annually and have reviewed hundreds of papers over my career. I review primarily for *Physical Review B* and *Physical Review Letters*, but I also review regularly for the *Journal of Chemical Education*, *Philosophical Magazine*, *Nature*, *Nature Materials*, *Science*, and the *Journal Physical Chemistry*. I also review proposals, typically two or three per year, most often for NSF and AFOSR. I have sat on NSF and DOE review panels, most recently, a DOE review panel for “Future Generation of Photovoltaics.”

COMMITTEES AND PANELS

Chair, Materials Reliability subgroup of the National Academy Panel on Materials Science and Engineering 2008-2010

Board of Visitors, Army Research Office’s Chemistry Division, 2010-2012

National Academy Panel on Armor and Armaments, 2007-2012

Board of Visitors, Army Research Office’s Materials Science Division, 2007-2009

National Research Council’s planning committee for the workshop entitled *Toward Sustainable Critical Infrastructure Systems: Framing the Challenges* to be held March 2008

Organizing Committee, *International Conference on DFT in Materials Science*, Oran Algeria, May 2007

Organizing Committee, Colorado Energy Research Institute’s 26th Oil Shale Symposium, Golden, Colorado, October 17-18, 2006

Organizing committee, *NATO Advanced Research Workshop on the Chemistry and Physics of Fracture*, Bad Reichenhall, F.R. Germany, June 1986

SYMPOSIA

Symposium Organizer, *Theory Assisted Materials Design*, MRS Fall Meeting, Boston, Massachusetts, December 1997

PROFESSIONAL ACTIVITIES—CONSULTING

Trek Bicycles, 2010

La Plata County, Colorado, 2010

Permanent Subcommittee on Investigations, United States Senate, 2007-2009

Tecplot, Seattle, Washington, 2006-

Nova and WGBH, Boston, Massachusetts, 2004-2006

Progress Energy, Raleigh, North Carolina, 2003-2005
Questek Innovations, Evanston, Illinois, 2002-present
United Technologies Research Center, Hartford, Connecticut, 1990-2002
Dow-Corning Research Center, Midland, Michigan, 1997-2002
Martin Marietta Research Labs, Baltimore, Maryland, 1987-1990

CSM COMMITTEE SERVICE:

SCHOOL WIDE

President, CSM Faculty Senate (8/2009-8/2010)
Handbook Committee (2009 to 2010)
Chair, Committee on Committees (2009-2010)
Research Management Cabinet (2008 to 2009)
Web Redesign Committee (5/2007 to 9/2008)
McBride Tutorial Committee (2004 to 2009)
Chair, Research Council (9/2007 to 9/2008)
Faculty Senate (9/2007 to 9/2008)
Faculty Senate (9/2003 to 9/2005)
Faculty Senate Executive Committee (9/2003 to 9/2004)
Faculty Senate Representative to Undergrad Council (9/2004 to 9/2005)
Technology Fee Committee (9/2002 to 9/2004)

DEPARTMENTAL

Member, Public Relations Committee (2013-present)
Member, Freshman Curriculum Committee (2012-present)
Chair, Senior Promotion and Tenure Committee (2012, 2013)
Chemistry's representative to the Research Council (2006-2008)
Chemistry's representative to the Materials Science Faculty Opportunities Committee (1998-2009)
Departmental Web Committee (1998-2011)
Search Committees (various)