

John W. Mintmire
Regents Professor and Head
Department of Physics
Oklahoma State University

145 Physical Sciences Bldg
Stillwater, OK 74078
(voice) 405.744.5796
(fax) 405.744.6811
(email) john.mintmire@okstate.edu
(web) <http://www.physics.okstate.edu/mintmire/>

1906 S Iba Drive
Stillwater, OK 74074
(home) 405.377.5390
(cell) 405.612.5163

Education

- Ph. D. in physics, 1976-1980, University of Florida, Gainesville, Florida
Dissertation: "LCAO Local Density Functional Approach to Surface Electronic Surface Calculations"
- B. S. in physics, 1972-1976, University of Florida, Gainesville, Florida

Professional Career

- Regents Professor (2009-), Professor (2001-2009), Department of Physics, Oklahoma State University
- Head (2001-2003,2011-), Interim Head (2010-2011), Department of Physics, Oklahoma State University
 - Supervise department of 23 tenure-track faculty, 8 staff with annual operating budget of about \$3M
 - Oversee faculty reappointment, promotion, and tenure process, as well as annual performance appraisal process
 - Administered NSF IGERT grant supporting interdisciplinary photonics program shared between physics, electrical engineering, and chemistry departments (2002-2004)
 - Acted as Department liaison with College of Engineering, Architecture, and Technology ABET accreditation review
- Associate Dean of Research (2004-2006), Interim Associate Dean (2003-2004), College of Arts and Sciences, Oklahoma State University
 - Supervised College Office of Research Support, supporting proposal preparation for extramural funding, post-award handling
 - Coordinated startup funding for new faculty hires and cost-share funding for grants
 - Administered internal college competitive grant programs for scholarly travel and other activities for all 24 departments across college
- Research Physicist (1983-2001), Chemistry Division, US Naval Research Laboratory, Washington, DC
 - Developed forefront research program in computational physics and chemistry of low-dimensional materials
 - Made major contributions to early theoretical understanding of carbon nanotube materials

Other Professional Appointments

- Program Director (2008-2009), Condensed Matter and Materials Theory Program, Division of Materials Research, National Science Foundation, Arlington, VA
- Program Director (1998-1999), Materials Theory Program, Division of Materials Research, National Science Foundation, Arlington, VA
- Visiting Associate Professor (1989-1990), Department of Physics, Ohio State University, Columbus, OH
- National Research Council (1981-1983) Postdoctoral Research Fellow, Chemistry Division, Naval Research Laboratory, Washington, DC
- Postdoctoral Associate (1980-1981), Quantum Theory Project, University of Florida, Gainesville, FL

Professional Societies and Activities

American Physical Society (Fellow)

American Chemical Society

Materials Research Society

International Union of Pure and Applied Chemistry (Fellow)

Sigma Xi

Editorial Board, International Journal of Quantum Chemistry

Editorial Board, Advances in Quantum Chemistry

Courses Taught

Oklahoma State University

[F: Fall semester, S: Spring semester, Su: Summer term]

PHYS 3013, Classical Mechanics I (S 2002)

PHYS 5960, Problems in Chemical Physics (Su 2003, F 2007)

PHYS 4003, Computational Physics (F 2003, F2006)

PHYS 5453, Methods of Theoretical Physics (F 2008, F2009, F2010)

PHYS 5663, Solid State I (S 2007, S 2008, S2010)

PHYS 5713, Solid State II (F 2004)

PHYS 4010, Mathematical Methods for Geophysics [special topics] (F 2011)

Graduate Student Degrees Advised

Pavan Pillalamarri, Ph.D., physics, estimated graduation date, May 2012
Vasantha Jogireddy, Ph.D., physics, May 2011
Junwen Li, Ph.D., physics, May 2010
Shelly Elizondo, Ph.D., photonics, August 2006; M.S., photonics, May 2005.
Ben Landis, M.S., physics, December 2005.
Marty Monigold, M.S., photonics, May 2005.
John Kernal, M.S., photonics, August 2003.

Undergraduate Students Advised

Markus Vasquez (Oklahoma State University), 2008-2009 [OSU Niblack Scholar]
Andrew Lau (Oklahoma Baptist University), 2005 [OSU Physics REU]
J. Thomas Alford (Northwestern University), 2004 [OSU Physics REU]
Shagoto Nandi (Boston University), 2004 [OSU Physics REU]
Jacob Weierman (Oklahoma State University), 2003 [OSU Physics REU]

Honors and Awards

Oklahoma State University Regents Distinguished Research Award, 2010
College of Liberal Arts and Sciences (CLAS) Outstanding Alumni Award, University of Florida, October 2005
Fellow, International Union of Pure & Applied Chemistry, January 2002
Fellow, American Physical Society, Division of Materials Physics, November 19, 2000
Finalist, Foresight Institute Feynman Award (Theoretical) in Nanotechnology, 2000
NRL Research Publication Awards, 1983, 1991
NSF Graduate Fellowship, University of Florida (1976-1979)

External Grant Support (OSU)

- “Nanoscale Modeling of Tribological Processes in Extreme Conditions”, J. W. Mintmire and Y. Guo, DoD EPSCoR Program, July 2007-June 2011, \$360,000
- “Optoelectronic Properties of Carbon Nanostructures”, J. W. Mintmire, DOE EPSCoR State-National Lab Partnership Program, DOE Grant DE-FG02-07ER46362, Feb 2007-Jan 2011, \$450,000
- “Research Support for DoD HPCMO CHSSI Project: Computational Tools for Nanoscale Materials Design”, Naval Research Laboratory, July 2003-June 2006, \$300,000
- “Computational Modeling for Inorganic Nanowires”, Oklahoma NASA EPSCoR Research Initiation Grant, February 2004-July 2004, \$18,939
- “Research Support for DoD HPCMO CHSSI CCM-5: Molecular Dynamics of Energetic and Nonenergetic Materials”, Office of Naval Research, August 2002-November 2003, \$40,000
- “Computational Materials Physics of Helical Nanostructures”, J. W. Mintmire, Office of Naval Research, Dec 2001-May 2005, \$160,000
- “IGERT: Advanced Graduate Training in Photonics Research”, J. W. Mintmire, J. J. Song, M. A. Soderstrand, N.A. Kotov, and J. Krasinski, National Science Foundation, September 2001-September 2004, \$1,492,502

External Grant Support (NRL)

- “Molecular Dynamics for Energetic & Nonenergetic Materials”, J. W. Mintmire, C. T. White, M. L. Elert, and J. A. Harrison, Jan 2000-Sep 2002, DoD HPCMO CHSSI program, \$390,000
- “Simulations of Reactive Collisions in Detonating Solids”, J. W. Mintmire, C. T. White, and B. I. Dunlap, Apr 1999-Sep 2000, Office of Naval Research, \$150,000
- “Theoretical Chemistry of Low-Dimensional Materials”, J. W. Mintmire and C. T. White, Oct 1999-Sep 2001, Office of Naval Research, \$255,000
- “First-Principles Molecular-Dynamics Simulations of Tribology,” J. W. Mintmire, B. I. Dunlap, and C. T. White, Jan 1995-Sep 2001, Office of Naval Research, \$540,000
- “Theoretical Chemistry of Group IV and Low-Dimensional Materials,” with C. T. White, Oct 1994-Sep 1999, Office of Naval Research, \$540,000
- “Molecular Dynamics Simulations of Reactive Collisions in Detonating Solids,” D.W. Brenner, J W. Mintmire, D. H. Robertson, and C. T. White, Oct 1992-Sep 1995, Office of Naval Research, 330,000
- “Chemistry of Group IV Materials,” J. W. Mintmire, D. L. Venezky, D. W. Brenner, and C. T. White, Oct 1991-Sep 1994, Office of Naval Research, \$330,000
- “Simulations of Chemical Wear at Diamond Interfaces,” D. W. Brenner, J. W. Mintmire, and C. T. White, Oct 1990-Sep 1991, Office of Naval Research, \$40,000
- “Chemistry of Silicon in Polymers and Interfaces,” J. W. Mintmire, B. I. Dunlap, and C. T. White, Jun 1990-Sep 1991, Office of Naval Research, \$26,000
- “Model Studies of Composition-Modulated Metal Alloys,” J. W. Mintmire and D. W. Brenner, Apr 1988-Sep 1989, Office of Naval Research, \$55,000

Papers in Refereed Journals:

101. “Robust ballistic transport in narrow armchair-edge graphene nanoribbons with chemical edge disorder”, D. Gunlycke, J. W. Mintmire, and C. T. White, *J. Phys. Chem. Lett.* **1**, 1082-1085 (2010).
100. “Edges bring new dimension to graphene nanoribbons”, D. Gunlycke, J. W. Li, J. W. Mintmire, and C. T. White, *Nano Lett.* **10**, 3638-3643 (2010).
99. “Electronic transport of silicon nanowires with surface defects”, J. W. Li, T. Jayasekera, V. Meunier, and J. W. Mintmire, *Int. J. Quantum Chem.* **109**, 3705-3710 (2009). [DOI: [10.1002/qua.22342](https://doi.org/10.1002/qua.22342)]
98. “Multiscale Modeling of Metal-Metal Contact Dynamics Under High Electromagnetic Stress: Timescales and Mechanisms for Joule Melting of Al-Cu Asperities”, D. L. Irving, C. W. Padgett, Y. Guo, J. W. Mintmire, and D. W. Brenner, *IEEE Trans. Magn.* **45**, 331-335 (2009).
97. “First-Principles Simulations of Chiral Double-Wall Carbon Nanotubes”, T. Jayasekera, B. A. Landis, and J. W. Mintmire, *Int. J. Quantum Chem.* **108**, 2943. (2008) [DOI: [10.1002/qua.21888](https://doi.org/10.1002/qua.21888)]
96. “Effect of Phase Breaking Events on Electron Transport in Mesoscopic and Nano Devices”, T. Jayasekera, P. Pillalamarri, J. W. Mintmire, and V. Meunier, *Int. J. Quantum Chem.* **108**, 2896 (2008). [DOI: [10.1002/qua.21834](https://doi.org/10.1002/qua.21834)]
95. “Graphene Nanostrip Digital Memory Device”, D. Gunlycke, D. A. Areshkin, J. W. Li, J. W. Mintmire, and C. T. White, *Nano Lett.* **7**, 3608-3611 (2007). [DOI: [10.1021/nl0717917](https://doi.org/10.1021/nl0717917)]
94. “First-Principles Study of the Optical Properties of ZnO Single-Wall Nanotubes”, S. L. Elizondo and J. W. Mintmire, *J. Phys. Chem. C* **111**, 17821-17826 (2007). [DOI: [10.1021/jp071319+](https://doi.org/10.1021/jp071319+)]
93. “First-Principles Properties of Organic Polymer Photovoltaic Materials”, T. Jayasekera, M. S. Monigold, S. L. Elizondo, and J. W. Mintmire, *Int. J. Quantum Chem.* **107**, 3120-3125 (2007). [DOI: [10.1002/qua.21443](https://doi.org/10.1002/qua.21443)]
92. “Lattice Vacancy Effects on Electron Transport in Multiterminal Graphene Nanodevices”, T. Jayasekera and J. W. Mintmire, *Int. J. Quantum Chem.* **107**, 3071-3076 (2007). [DOI: [10.1002/qua.21437](https://doi.org/10.1002/qua.21437)]
91. “Altering Low-Bias Transport in Zigzag-Edge Graphene Nanostrips with Edge Chemistry”, D. Gunlycke, J. W. Li, J. W. Mintmire, and C. T. White, *Appl. Phys. Lett.* **91**, 112108 (2007). [DOI: [10.1063/1.2783196](https://doi.org/10.1063/1.2783196)]
90. “Transport in Multiterminal Graphene Nanodevices”, T. Jayasekera and J. W. Mintmire, *Nanotechnology* **18**, 424033 (2007). [DOI: [10.1088/0957-4484/18/42/424033](https://doi.org/10.1088/0957-4484/18/42/424033)]
89. “Hidden One-Electron Interactions in Carbon Nanotubes Revealed in Graphene Nanostrips”, C. T. White, J. Li, D. Gunlycke, and J. W. Mintmire, *Nano Lett.* **7**, 825 (2007).
88. “Helical Strain in Carbon Nanotubes: Speed of Sound and Poisson Ratio from First Principles”, H. M. Lawler, J. W. Mintmire, and C. T. White, *Phys. Rev. B* **74**, 125415 (2006).
87. “Endohedral Carbon Chains in Chiral Single-Wall Carbon Nanotubes”, R. K. Vadapalli and J. W. Mintmire, *Int. J. Quantum Chem.* **106**, 2326-2330 (2006).

86. “Ab Initio Study of Helical Silver Single-Wall Nanotubes”, S. L. Elizondo and J. W. Mintmire, *Phys. Rev. B* **73**, 045431 (2006).
85. “Radial-Breathing Mode Frequencies for Single-Walled Carbon Nanotubes of Arbitrary Chirality: First-Principles Calculations”, H. M. Lawler, D. Areshkin, J. W. Mintmire, and C. T. White, *Phys. Rev. B* **72**, 233403 (2005). [DOI [10.1103/PhysRevB.72.233403](https://doi.org/10.1103/PhysRevB.72.233403)]
84. “Simulations of Metal Nanowires”, S. L. Elizondo and J. W. Mintmire, *Int. J. Quantum Chem.* **105**, 772-780 (2005). [DOI [10.1002/qua.20661](https://doi.org/10.1002/qua.20661)]
83. “Molecular Dynamics Simulations of the Oxidation of Aluminum Nanoparticles”, S. Alavi, J. W. Mintmire, and D. L. Thompson, *J. Phys. Chem. B* **109**, 209-214 (2005). [DOI [10.1021/jp046196x](https://doi.org/10.1021/jp046196x)]
82. “Theoretical Elastic Properties of Single Walled Carbon Nanotubes”, J. T. Alford, B. A. Landis, and J. W. Mintmire, *Int. J. Quantum Chem.* **105**, 767-771 (2005). [DOI [10.1002/qua.20660](https://doi.org/10.1002/qua.20660)]
81. “Density-Functional Study of the Mechanical and Electronic Properties of Narrow Carbon Nanotubes under Axial Stress”, F. Bogar, T. Mezo, J. W. Mintmire, F. Bartha, and C. Van Alsenoy, *Phys. Rev. B* **72**, 085452 (2005).
80. “Fundamental Properties of Single-Wall Carbon Nanotubes”, C. T. White and J. W. Mintmire, *J. Phys. Chem. B* **109**, 52-65 (2005) [DOI [10.1021/jp047416+](https://doi.org/10.1021/jp047416+)]
79. “Reactive Bond-Order Simulations Using Both Spatial and Temporal Approaches to Parallelism”, S. J. Stuart, Y. Li, O. Kum, J. W. Mintmire, and A. F. Voter, *Structural Chemistry* **15**, 483-491 (2004).
78. “Stability and Electronic Structure of Phosphorus Nanotubes”, I. Cabria and J. W. Mintmire, *Europhys. Lett.* **65**, 82-88 (2004).
77. “Metallic and Semiconducting Narrow Carbon Nanotubes”, I. Cabria, J. W. Mintmire, and C. T. White, *Phys. Rev. B* **67**, R121406 (2003).
76. “Stability of Narrow Zigzag Carbon Nanotubes”, I. Cabria, J. W. Mintmire, and C. T. White, *Int. J. Quantum Chem.* **91**, 51-56 (2003).
75. “Efficient Parallel Algorithms for Molecular Dynamics Simulations Using Variable Charge Transfer Electrostatic Potentials”, D. J. Keffer and J. W. Mintmire, *Int. J. Quantum Chem.* **80**, 733-742 (2000).
74. “Endohedral Selenium Chains in Carbon, Boron Nitride, and BC₂N Nanotubes”, R. A. Jishi, C. T. White, and J. W. Mintmire, *Int. J. Quantum Chem.* **80**, 480-485 (2000).
73. “Detonation Hugoniot from Molecular Dynamics Simulations”, D. R. Swanson, J. W. Mintmire, D. H. Robertson, and C. T. White, *Chem. Phys. Rep.* **18**, 1871-1882 (2000).
72. “Local Density Approximation Calculation of the Conformation and Electronic Structure of Poly(fluoroethylene)s”, M. S. Miao, M.-L. Zhang, V. E. Van Doren, J. J. Ladik, and J. W. Mintmire, *J. Phys. Chem. A* **104**, 6809-6816 (2000).
71. “Calculation of the Total Energy per Unit Cell and of the Band Structures of the Five Nucleotide Base Stacks Using the Local Density Approximation”, M.-L. Zhang, M. S. Miao, V. E. Van Doren, J. J. Ladik, and J. W. Mintmire, *J. Chem. Phys.* **111**, 8696 (1999).
70. “Energetics of Aluminum Vacancies in γ -Alumina”, F. H. Streitz and J. W. Mintmire, *Phys. Rev. B* **60**, 773 (1999).

69. "First-Principles Calculation of the Conformation and Electronic Structure of Polyparaphenylene", M. S. Miao, P. E. Van Camp, V. E. Van Doren, J. J. Ladik, and J. W. Mintmire, *J. Chem. Phys.* **109**, 9623 (1998).
68. "Peptide Nanotubes: an Inert Environment", R. A. Jishi, N. C. Braier, C. T. White, and J. W. Mintmire, *Phys. Rev. B* **58**, R16009 (1998).
67. "Universal Density of States for Carbon Nanotubes", J. W. Mintmire and C. T. White, *Phys. Rev. Lett.* **81**, 2506 (1998).
66. "First-Principles Band Structures of Armchair Nanotubes", J. W. Mintmire and C. T. White, *Appl. Phys. A* **67**, 65 (1998).
65. "Density of States Reflects Diameter in Nanotubes", C. T. White and J. W. Mintmire, *Nature* **394**, 29 (1998).
64. "Atomic Simulations of Shock Induced Pore Collapse in Model Materials", J. W. Mintmire, J. J. C. Barrett, D. H. Robertson, and C. T. White, *Chem. Phys. Rep.* **17**, 37-46 (1998) [*Khim. Fiz.* **17**, 30 (1998)].
63. "First Principles Simulations of Endohedral Bromine in BC₃", R. A. Jishi, C. T. White, and J. W. Mintmire, *J. Phys. Chem. B* **102**, 1568 (1998).
62. "LDA Calculation of the Conformation and Electronic Structure of Polytetrafluorethylene", M.S. Miao, P. E. Van Camp, V. E. Van Doren, J. J. Ladik, and J. W. Mintmire, *Int. J. Quantum Chem.* **64**, 243 (1997).
61. "Conformation and Electronic Structure of Polyethylene: A Density Functional Approach", M. S. Miao, P. E. Van Camp, V. E. Van Doren, J. J. Ladik, and J. W. Mintmire, *Phys. Rev. B.* **54**, 10430 (1996).
60. "Molecular Dynamics Simulations of Elastic Response and Tensile Failure of Alumina", F. H. Streitz and J. W. Mintmire, *Langmuir* **12**, 4605 (1996).
59. "Fullerene Formation and Annealing", J. W. Mintmire, *Science* **272**, 45 (1996).
58. "Electronic Structure Simulations of Carbon Nanotubes", J. W. Mintmire and C. T. White, *Synth. Metals* **77**, 31 (1996).
57. "Electronic and Structural Properties of Carbon Nanotubes", J. W. Mintmire and C. T. White, *Carbon* **33**, 893 (1995).
56. "Metal/Oxide Interfaces: An Electrostatic-Based Model", F. H. Streitz and J. W. Mintmire, *Composite Interfaces* **2**, 473 (1994).
55. "Chemistry and Phase Transitions from Hypervelocity Impacts", C. T. White, S. B. Sinnott, J. W. Mintmire, D. W. Brenner, and D. H. Robertson, *Int. J. Quantum. Chem. Symp.* **28**, 129 (1994).
54. "Electrostatic Potentials for Metal Oxide Surfaces and Interfaces", F. H. Streitz and J. W. Mintmire, *Phys. Rev. B.* **50**, 11996-12003 (1994).
53. "Electrostatic-Based Model for Alumina Surfaces", F. H. Streitz and J. W. Mintmire, *Thin Solid Films* **253**, 179-184 (1994).
52. "Molecular Dynamics Simulation of Void Collapse in Shocked Model Molecular Solids", J. W. Mintmire, D. H. Robertson, and C. T. White, *Phys. Rev. B.* **49**, 14859-14864 (1994).
51. "Charge Transfer and Bonding in Metallic Oxides", F. H. Streitz and J. W. Mintmire, *J. Adhesion Sci. Technol.* **8**, 853-864 (1994).
50. "Properties of Fullerene Nanotubules", J. W. Mintmire, D. H. Robertson, and C. T. White, *J. Phys. Chem. Solids* **54**, 1835-1840 (1993).

49. "First-Principles Electronic Properties of Model Silicon-Based Quantum Wires", J. W. Mintmire, *J. Vac. Sci. Tech. A* **11**, 1733-1735 (1993).
48. "Helical and Rotational Symmetries of Nanoscale Graphitic Tubules", C. T. White, D. H. Robertson, and J. W. Mintmire, *Phys. Rev. B.* **47**, 5485-5488 (1993).
47. "Are Fullerene Tubules Metallic?" J. W. Mintmire, B. I. Dunlap, and C. T. White, *Phys. Rev. Lett.* **68**, 631 (1992).
46. "Possible Many-Body Effects in Scanning-Tunneling Microscopy of Molecular Adsorbates", J. W. Mintmire, J. A. Harrison, R. J. Colton, and C. T. White, *J. Vac. Sci. Technol. A* **10**, 603 (1992).
45. "Structural and Elastic Properties of Transition-Metal Superlattices", R. S. Jones, J. A. Slotwinski, and J. W. Mintmire, *Phys. Rev. B.* **45**, 13624-13630 (1992).
44. "Energetics of Nanoscale Graphitic Tubules", D. H. Robertson, D. W. Brenner and J. W. Mintmire, *Phys. Rev. B. (Rapid Comm.)* **45**, 12592-12595 (1992).
43. "Local-Density Functional Photoelectron Spectra of Fullerenes", J. W. Mintmire, B. I. Dunlap, D. W. Brenner, R. C. Mowrey, and C. T. White, *Phys. Rev. B (Rapid Comm.)* **43**, 14281 (1991).
42. "Geometric and Electronic Structures of C₆₀H₆₀, C₆₀F₆₀, and C₆₀H₃₆", B. I. Dunlap, D. W. Brenner, J. W. Mintmire, R. C. Mowrey, and C. T. White, *J. Phys. Chem.* **95**, 5763 (1991).
41. "Simulations of C₆₀ Collisions with a Hydrogen-Terminated Diamond (111) Surface", R. C. Mowrey, D. W. Brenner, B. I. Dunlap, J. W. Mintmire, and C. T. White, *J. Phys. Chem.* **95**, 7138 (1991).
40. "Local Density Functional Electronic Structures of Three Stable Icosahedral Fullerenes", B. I. Dunlap, D. W. Brenner, J. W. Mintmire, R. C. Mowrey, and C. T. White, *J. Phys. Chem.* **95**, 8737 (1991).
39. "Group IV Covalent Clusters: Si₄₅ and C₄₄ and C₄₅", D. W. Brenner, B. I. Dunlap, J. A. Harrison, J. W. Mintmire, R. C. Mowrey, D. H. Robertson, and C. T. White, *Phys. Rev. B. (Rapid Comm.)* **44**, 3479 (1991).
38. "Ground State and Vertical Ionization Energies Versus Si-Si-Si and C-C-C Bond Angles in Si₃H₈ and C₃H₈", J. V. Ortiz and J. W. Mintmire, *J. Phys. Chem.* **95**, 8609 (1991).
37. "D-D (H-H) Interactions within the Interstices of Pd", C. T. White, D. W. Brenner, R. C. Mowrey, J. W. Mintmire, P.P. Schmidt, and B. I. Dunlap, *Jap. J. Appl. Phys.* **30**, 182-189 (1991).
36. "Linear Combination of Gaussian-type Orbitals Local-Density-Functional Cluster Studies of D-D-Interactions in Titanium and Palladium", B. I. Dunlap, D. W. Brenner, R. C. Mowrey, J. W. Mintmire, and C. T. White, *Phys. Rev. B* **41**, 9683 (1990).
35. "Model Studies of Composition-Modulated Cu-Ni Superlattices", J. W. Mintmire, *Mater. Sci. Eng.* **A126**, 29-31 (1990).
34. "Limits of Chemical Effects on Cold Fusion", C. T. White, B. I. Dunlap, D. W. Brenner, R. C. Mowrey, and J. W. Mintmire, *J. Fusion Energy* **9**, 363-366 (1990).
33. "Geometry Optimization of Molecules Within an LCGTO Local-Density Functional Approach", J. W. Mintmire, *Int. J. Quantum Chem. Symp.* **24**, 851-857 (1990).

32. "Local-Density-Functional Total Energy Gradients in the Linear-Combination-of-Gaussian-Type-Orbitals Method", B. I. Dunlap, J. Andzelm, and J. W. Mintmire, *Phys. Rev. A* **42**, 6354-6359 (1990).
31. "Conformational Effects in Organopolysilanes: A First-Principles Approach", J. W. Mintmire, *Phys. Rev. B* **39**, 13350 (1989).
30. "Chemical Forces Associated with Deuterium Confinement in Palladium", J. W. Mintmire, B. I. Dunlap, D. W. Brenner, R. C. Mowrey, H. D. Ladouceur, P. P. Schmidt, C. T. White, and W. E. O'Grady, *Phys. Lett. A* **138**, 51-54 (1989).
29. "Comment on 'Ground State of trans-Polyacetylene and the Peierls Mechanism'", J. W. Mintmire and C. T. White, *Phys. Rev. Lett.* **63**, 2532 (1989).
28. "Conformation and Electronic Structure of Heterocyclic Chain Polymers", J. W. Mintmire, C. T. White, and M. L. Elert, *Synth. Metals* **25**, 109 (1988).
27. "Ground States and Ionization Energies of Si₂H₆, Si₃H₈, Si₅H₁₂", J. V. Ortiz and J. W. Mintmire, *J. Am. Chem. Soc.* **110**, 4522 (1988).
26. "Geometry Optimization Using Local-Density Functional Methods: Numerical Aspects", R.S. Jones, J. W. Mintmire, and B. I. Dunlap, *Int. J. Quantum Chem. Symp.* **22**, 77 (1988).
25. "Ab Initio Conformation and Ionization Potentials of Polysilane Oligomers", J. W. Mintmire, and J. V. Ortiz, *Macromolecules* **21**, 1189 (1988).
24. "Local-Density Functional Results for the Dimerization of trans-Polyacetylene: Relationship to the Band Gap Problem", J. W. Mintmire and C. T. White, *Phys Rev. B* **35**, 4180 (1987).
23. "Photoelectron Spectra From Local-Density Functional Calculations: Application to Chain Polymers", J. W. Mintmire, F.W. Kutzler, and C. T. White, *Phys. Rev. B* **36**, 3312 (1987).
22. "Brillouin Zone Treatment in Total Energy Calculations of Peierls Distorted Chains", J. W. Mintmire and C. T. White, *Int. J. Quantum Chem. Symp.* **21**, 131 (1987).
21. "Preliminary Report on a Local-Density Functional Study of Polysilane Chains", J. W. Mintmire, *Int. J. Quantum Chem. Symp.* **21**, 761 (1987).
20. "Theoretical Photoelectron Spectra Using Local-Density Functional Results", J. W. Mintmire, F.W. Kutzler, and C. T. White, *Int. J. Quantum Chem. Symp.* **19**, 745 (1986).
19. "Soliton Defects in Polyacetylene: Local-Density Functional Results", F.W. Kutzler, C. T. White, and J. W. Mintmire, *Int. J. Quantum Chem.* **29**, 793 (1986).
18. "Heteroatom Effects in Heterocyclic Ring Chain Polymers", J. W. Mintmire, C. T. White, and M. L. Elert, *Synth. Metals* **16**, 235 (1986).
17. "Conformation and Electronic Properties of Helical cis-Polyacetylene", M. L. Elert, C. T. White, and J. W. Mintmire, *Mol. Cryst.* **125**, 329 (1985).
16. "Local-Density Functional Approach to Chain Polymers", J. W. Mintmire, C. T. White, and M. L. Elert, *Mol. Cryst.* **125**, 337 (1985).
15. "X α Approach for the Determination of Electronic and Geometric Structure of Polyacetylene and Other Chain Polymers", J. W. Mintmire and C. T. White, *Phys. Rev. Lett.* **50**, 101 (1983).
14. "Theoretical Treatment of the Dielectric Response of all-trans Polyacetylene", J.W. Mintmire and C. T. White, *Phys. Rev. B* **27**, 1447 (1983).

13. "Local-Density Functional Approach to all-trans Polyacetylene", J. W. Mintmire and C. T. White, *Phys. Rev. B* **28**, 3283 (1983).
12. "Dielectric Properties of Polyacetylene", J. W. Mintmire, C. T. White, and D. L. Peebles, *J. Phys. (Paris), Colloq.* **44(C3)**, 507 (1983).
11. "Effects of Off-Diagonal Disorder on Soliton-and Polaron-like States in trans-Polyacetylene", C. T. White, M. L. Elert, and J. W. Mintmire, *J. Phys. (Paris), Colloq.* **44 (C3)**, 507 (1983).
10. "Tight-Binding Studies for Electroactive Organic Polymers", M. L. Elert, J. W. Mintmire and C. T. White, *J. Phys. (Paris), Colloq.* **44(C3)**, 451, (1983).
9. "Theoretical Photoelectron Cross-Sections for Chain Polymers", J. W. Mintmire and C. T. White, *Int. J. Quantum Chem. Symp.* **17**, 609 (1983).
8. "Charge Transfer in Na₂AsF₆ Intercalated Graphite", L. Mattix, J. Milliken, H. A. Resing, J. W. Mintmire, and D. C. Weber, *Synth. Metal* **8**, 177 (1983).
7. "A Comparison of the LCAO-X α Method with the Hartree-Fock and Multiple-Scattering X α methods on Carbon Monoxide", J. W. Mintmire and J. R. Sabin, *Chem. Phys.* **51**, 91 (1980).
6. "Local Density Functional Methods in Two-Dimensionally Periodic Systems: I. The Atomic Hydrogen Monolayer", J. W. Mintmire and J. R. Sabin, *Int. J. Quantum Chem. Symp.* **14**, 707 (1980).
5. "Fitting the Coulomb Potential Variationally in Linear Combination of Atomic Orbitals Density Functional Calculations", J. W. Mintmire and B. I. Dunlap, *Phys. Rev. A* **25**, 88 (1982).
4. "Model Study of the Effects of Correlations on the XVV-Auger Lineshape of Chemisorbed Species", C. T. White, J. W. Mintmire, and E. N. Economou, *J. Vac. Sci. Technol.* **20**, 565 (1982).
3. "Local Density Functional Methods in Two-Dimensionally Periodic Systems. Hydrogen and Beryllium Monolayers", J. W. Mintmire, J. R. Sabin, and S. B. Trickey, *Phys. Rev. B* **26**, 1743 (1982).
2. "LCAO Methods in the X α Formalism: A Comparison of Results for the F₂ Molecule", J.W. Mintmire, *Int. J. Quantum Chem. Symp.* **13**, 163 (1979).
1. "Intermolecular Potential Studies of Hydrogen Interactions with Rare-Gas Atoms", J. W. Mintmire and J. R. Sabin, *Int. J. Quantum Chem. Symp.* **10**, 213 (1976).

Books and Chapters in Books

12. "Single-Walled Carbon Nanotubes: Structures and Symmetries", C. T. White and J. W. Mintmire, in *Dekker Encyclopedia of Nanoscience and Nanotechnology*, Eds., J. A. Schwarz, C. I. Contescu, and K. Putyera, (Dekker, 2004), pp. 3629-3639.
11. "An Object-Oriented Framework for Parallel, Reactive Molecular Dynamics", S.J. Stuart, Y. Li, S. B. Gowda, H. Sanghavi and J. W. Mintmire, in *Parallel and Distributed Computing and Systems*, (Acta Press, Anaheim, CA), pp. 476-482 (2002).
10. "Density Functional Simulations of Carbon Nanotubes", J. W. Mintmire and C. T. White, in *Density Functional Theory and its Application to Materials*, Eds., V. Van Doren, C. Van Alsenoy, and P. Geerlings, AIP Conf. Proc. Vol. 577, (AIP, Melville, NY, 2001), pp. 98-116.
9. "Electronic Structure of Conducting Carbon Nanotubes", J. W. Mintmire, R. A. Jishi and C. T. White, in *Designing Novel Materials*, Eds., B. K. Rao and S. N. Behera, (Nova, New York, 1998), p. 319.
8. "Properties: Theoretical Predictions", J. W. Mintmire and C. T. White, in *Carbon Nanotubes: Preparation and Properties*, Ed., T.W. Ebbesen, (CRC Press, Boca Raton, 1997), pp. 191-224.
7. "LDF Electronic Structure of Fullerene Tubules", J. W. Mintmire, in *Electronic Density Functional Theory of Molecules, Clusters, and Solids*, Ed. D.E. Ellis, (Kluwer, 1995), pp. 153-175.
6. "Science and Technology of Fullerene Materials, Eds., P. Bernier, D.S. Bethune, L.Y. Chiang, T. W. Ebbesen, R.M. Metzger and J. W. Mintmire, MRS Symposia Proceedings No. 359 (Materials Research Society, Pittsburgh, PA, 1995).
5. "Predicting Properties of Fullerenes and Their Derivatives", C. T. White, J. W. Mintmire, R. C. Mowrey, D. W. Brenner, D. H. Robertson, J.A. Harrison and B. I. Dunlap, in *Buckminsterfullerenes*; Eds., W.E. Billups and M. Ciufolini, (VCH, 1993), pp. 125-184.
4. "First-Principles Properties of Fullerene Tubules", J. W. Mintmire, D. H. Robertson and C. T. White, in *Fullerenes: Recent Advances in the Chemistry and Physics of Fullerenes*, Eds., K. Kadish and R.S. Ruoff, (The Electrochemical Society, Pennington, NJ, 1994), p. 286.
3. "Local-Density Functional Electronic Structure of Helical Chain Polymers", J. W. Mintmire, in *Density Functional Theory Approaches to Chemistry*, J.K. Labanowski and J. W. Andzelm, Eds. (Springer-Verlag, New York, 1991), pp. 125-137.
2. "Band Structure and Optical Absorption Properties of Polysilane Chains", J. W. Mintmire and J. V. Ortiz, in *Silicon-Based Polymer Science*; J.M. Zeigler and F.W.G. Fearon, Eds.; *Adv. Chem. Ser.* **224** (American Chemical Society, 1990) pp. 543-550.
1. "Ground States and Ionization Energies of Polysilane Oligomers", J. V. Ortiz and J. W. Mintmire, in *Silicon-Based Polymer Science*, J.M. Zeigler and F.W.G. Fearon, Eds., *Adv. Chem. Ser.* **224** (American Chemical Society, 1990) pp. 551-561.

Refereed Proceedings and Other Publications

32. “Radial-Breathing Mode Frequencies for Single-Walled Carbon Nanotubes of Arbitrary Chirality: First-Principles Calculations”, H. M. Lawler, J. W. Mintmire, D. A. Areshkin, and C. T. White, in *Dynamics in Small Confining Systems VIII*, edited by John T. Fourkas, Pierre Levitz, René Overney, Michael Urbakh (Mater. Res. Soc. Symp. Proc. 899E, Warrendale, PA, 2006), 0899-N07-25.
31. “First-Principles Study of Helical Silver Single-Wall Nanotubes and Nanowires”, S. L. Elizondo and J. W. Mintmire, in *Nanoparticles and Nanostructures in Sensors and Catalysis*, edited by Chuan-Jian Zhong, Nicholas A. Kotov, Wayne Daniell, Francis P. Zamborini (Mater. Res. Soc. Symp. Proc. 900E, Warrendale, PA, 2006), 0900-O12-04.
30. “Largest Band Gap of All Single-Walled Carbon Nanotubes”, I. Cabria, J. W. Mintmire, and C. T. White, in *Nanotube Based Devices*, Eds., P. Bernier, D. Carroll, G.-T. Kim, and S. Roth, MRS Symposia Proceedings No. 772 (Materials Research Society, Pittsburgh, PA, 2003), p. 121.
29. “Carbon Nanotubes: Experiments Catch Up with Theory”, C. T. White and J. W. Mintmire, 1999 NRL Review, pp. 87-89.
28. “Atomic-Scale Simulations of Structural Properties of Ceramics”, D. J. Keffer, F. H. Streitz and J. W. Mintmire, in *Solid-State Chemistry of Inorganic Materials*, Eds., A. Jacobson, P. Davies, T. Vanderah and C. T. Torardi, MRS Symposia Proceedings No. 453, (Materials Research Society, Pittsburgh, PA, 1997) 209.
27. “Molecular Dynamics Study of Chemistry from Strong Shock Waves Interacting with Voids”, C. T. White, J. J. C. Barrett, J. W. Mintmire, M. L. Elert and D. H. Robertson, in *Shock Compression of Condensed Matter-1995*, Eds., S.C. Schmidt and W.C. Tao, AIP Conference Proceedings 370 (AIP, Woodbury, 1996), pp. 187-190.
26. “Effects of Nanoscale Voids on the Sensitivity of Model Energetic Materials”, C. T. White, J. J. C. Barrett, J. W. Mintmire, M. L. Elert and D. H. Robertson, MRS Symposia Proceedings No. 418 (Materials Research Society, Pittsburgh, PA, 1996), p. 277.
25. “Atomic Scale Simulations of Tensile Failure in Metal Oxides”, F. H. Streitz and J. W. Mintmire, in *Structure and Properties of Interfaces in Ceramics*, Eds., D. A. Bonnell, U. Chowdhry and M. Rühle, MRS Symposia Proceedings No. 357 (Materials Research Society, Pittsburgh, PA, 1995) , pp. 459-463.
24. “Atomic Scale Failure of Tensile Failure in Metal Oxides”, F. H. Streitz and J. W. Mintmire, in *Structure and Properties of Interfaces in Ceramics*, Eds., D. A. Bonnell, U. Chowdhry and M. Rühle, MRS Symposia Proceedings No. 357 (Materials Research Society, Pittsburgh, PA, 1995), pp. 459-463.
23. “Electrostatic Potentials for Metal Oxide Surfaces and Interfaces”, F. H. Streitz and J. W. Mintmire, in *Interface Control of Electrical, Chemical, and Mechanical Properties*, Eds., S. P. Muraka, K. Rose, T. Ohmi and T. Seidel, MRS Symposia Proceedings No. 318 (Materials Research Society, Pittsburgh, PA, 1994), p. 679.

22. "Special C₄₄ Isomers", C. T. White, M. Lyons, D. W. Brenner, J. W. Mintmire, D. H. Robertson, R. C. Mowrey and B. I. Dunlap, in *Novel forms of Carbon II*, Eds., C. L. Renschler, D. Cox, J. Pouch and Y. Achiba, MRS Symposia Proceedings No. 349 (Materials Research Society, Pittsburgh, PA, 1994), p. 331.
21. "Molecular Dynamics of Void Collapse Mechanisms in Shocked Media", J. W. Mintmire, D. H. Robertson, M. L. Elert, D. W. Brenner and C. T. White, in *Shock Compression of Condensed Matter-1993*, Eds., S.C. Schmidt, J. W. Shaner, G.A. Samara and M. Ross, AIP Conference Proceedings Vol. 309, (AIP Press, 1994), pp. 969-972.
20. "Theory for New Carbon-Based Materials", D. W. Brenner, R. C. Mowrey, J. W. Mintmire, J.A. Harrison, D. H. Robertson, M. Lyons, B. I. Dunlap and C. T. White, in MRS Symposia Proceedings No. 270 (Materials Research Society, Pittsburgh, PA, 1993), p. 123.
19. "Dissociative Phase Transitions, Split Shock Waves, Rarefaction Shocks, and Detonation", C. T. White, D. H. Robertson, M. L. Elert, J. W. Mintmire and D. W. Brenner, in *Structure and Properties of Energetic Materials*, Eds., R. W. Armstrong and J. J. Gilman, MRS Symposia Proceedings No. 296 (Materials Research Society, Pittsburgh, PA, 1993), p. 123.
18. "Molecular Dynamics Simulations of Pressure Wave Effects at Voids in a Model Condensed-Phase Material", J. W. Mintmire, D. H. Robertson, D. W. Brenner and C. T. White, in *Shock Compression of Condensed Matter-1991*, Eds. R.O. Dick, J. W. Forbes and D.G. Tasker, (Elsevier, 1992) pp. 147-150.
17. "Relative Energies of C₄₄ Isomers", M. Lyons, B. I. Dunlap, D. W. Brenner, D. H. Robertson, R. C. Mowrey, J. W. Mintmire and C. T. White, *Physics and Chemistry of Finite Systems: From Cluster to Crystals*, P. Jena, S. N. Khanna and B.K. Rao (eds.) NATO ASI Series C **347** (Kluwer, Dordrecht) pp. 1347-1351 (1992).
16. "Virtual Symmetric Charge Transfer Superconducting Pairing Excitation in C₆₀", C. T. White, M.R. Cook, B. I. Dunlap, R. C. Mowrey, D. W. Brenner, P.P. Schmidt and J. W. Mintmire, *Physics and Chemistry of Finite Systems: From Cluster to Crystals*, P. Jena, S.N. Khanna and B.K. Rao (eds.) NATO ASI Series C **374** (Kluwer, Dordrecht) pp. 1397-1402 (1992).
15. "Molecular-Dynamics Simulations of C₆₀/He Collisions", R. C. Mowrey, D. W. Brenner, B. I. Dunlap, J. W. Mintmire and C. T. White, *Physics and Chemistry of Finite Systems From Clusters to Crystals*, P. Jena, S.N. Khanna and B.K. Rao (eds.) NATO ASI Series C **374** (Kluwer, Dordrecht) pp. 1353-1358 (1992)
14. "Workshop on Adhesion and Intermolecular Forces", J. W. Mintmire, B. I. Dunlap and C. T. White, NRL Memorandum Report, NRL/MR/6179-92-7143, September 18, 1992.
13. "Molecular Description of Chemically Sustained Shock Waves", C. T. White, D. H. Robertson, J. W. Mintmire, D. W. Brenner and M. L. Elert, *Revue Scientifique et Technique de la Defense* **16**, 157-160 (1992).

12. "Electronic Structure of Fullerene Tubules", J. W. Mintmire, D. H. Robertson, B. I. Dunlap, R. C. Mowrey, D. W. Brenner and C. T. White, in *Electrical, Optical, and Magnetic Properties of Organic Solid Materials*, Eds. L.Y. Chiang, A.F. Garito and D.J. Sandman, MRS Symposia Proceedings No. 247 (Materials Research Society Pittsburgh, PA, 1992) , pp. 339-343.
11. "Photoelectron Spectra of C₆₀H₃₆ and C₆₀H₆₀", B. I. Dunlap, J. W. Mintmire, D. H. Robertson, D. W. Brenner, R. C. Mowrey and C. T. White, in *Electric, Optical, and Magnetic Properties of Organic Solid Materials*, Eds. L. Y. Chiang, A. F. Garito, and D. J. Sandman, MRS Symposia Proceedings No. 247 (Materials Research Society Pittsburgh, PA, 1992), p. 351.
10. "First-Principles Simulations of Diamond Surface Formation via Radical Addition", J. W. Mintmire, D. W. Brenner, B. I. Dunlap, R. C. Mowrey and C. T. White, in *New Diamond Science and Technology, Proceedings of the 2nd Int. Conf. On New Diamond Sci. and Tech.*, Ed R. Messier and J. Glass, MRS International Conference Proceedings Series (Materials Research Society Pittsburgh, PA, 1991), p. 57.
9. "Molecular Simulations of the Reactions of Atomic Hydrogen with Diamond Surfaces", D. W. Brenner, B. I. Dunlap, J. W. Mintmire, R. C. Mowrey and C. T. White, in *New Diamond Science and Technology, Proceedings of the 2nd Int. Conf. On New Diamond Sci. and Tech.*, Ed R. Messier and J. Glass, MRS International Conference Proceedings Series (Materials Research Society Pittsburgh, PA, 1991), p. 39.
8. "Molecular Dynamics of Collisions of Buckminsterfullerene with Diamond Surfaces", R. C. Mowrey, D. W. Brenner, B. I. Dunlap, J. W. Mintmire and C. T. White in *Clusters and Cluster-Assembled Materials*, Eds. R. S. Averback, D. L. Nelson and J. Bernholc, MRS Symposia Proceedings No. 206 (Materials Research Society, Pittsburgh, PA 1991), pp. 357-362.
7. "First-Principles Study of Photoexcited Defects in Polysilane Chains", J. W. Mintmire, R. C. Mowrey, D. W. Brenner, B. I. Dunlap and C. T. White in *Defects in Materials*, Eds., P. D. Bristowe, J. E. Epperson, J. E. Griffith and Z. Liliental-Weber, MRS Symposia Proceedings No. 209 (Materials Research Society, Pittsburgh, PA, 1991).
6. "First-Principles Study of Soliton Hyperfine Interactions in Polyacetylene", C. T. White, F.W. Kutzler, J. W. Mintmire, and M. R. Cook, in *Defects in Materials*, Eds., P. D. Bristowe, J. E. Epperson, J. E. Griffith and Z. Liliental-Weber, MRS Symposia Proceedings No. 208 (Materials Research Society, Pittsburgh, PA, 1991).
5. "Possible Isomers and Electronic Structure of C₆₀H₃₆", B. I. Dunlap, D. W. Brenner, R. C. Mowrey, J. W. Mintmire, D. H. Robertson and C. T. White, in *Clusters and Cluster-Assembled Materials*, Eds., R.S. Averback, D.L. Nelson and J. Bernholc, MRS Symposia Proceedings No. 206 (Materials Research Society, Pittsburgh, PA, 1991) pp. 687-690.
4. "First-Principles Studies of Polysilane Model Systems", J. W. Mintmire and J. V. Ortiz, *Polym. Prepr.* 31, 234 (1990).

3. “Ground State and Vertical Ionization Energies Versus Si-Si-Si and C-C-C Bond Angles in Si_3H_8 and C_3H_8 ”, J. V. Ortiz and J. W. Mintmire, *Polym. Prepr*, **31**, 284 (1990).
2. “First-Principles Geometry Optimization of Polysilane”, J. W. Mintmire, *Mat. Res. Soc. Symp. Proc.* **141**, 235-239 (1989).
1. “Predicting the Properties of Chain Polymers”, C. T. White and J. W. Mintmire, NRL Review (1982).

Invited Talks at Professional Meetings and Workshops:

50. “Electronic and Transport Properties of Graphitic Nanostructures with Defects”, J. W. Mintmire, D. Gunlycke, and C. T. White, CECAM Workshop on Charge and Spin Transport in Chemically Modified Graphene Materials, Barcelona, Spain, April 7, 2011.
49. “Electronic Properties of Quasi-One-Dimensional Nanostructured Materials”, J. W. Mintmire, Functionalized Nanomaterials: Bio Helps Nano Workshop, Santa Fe, NM, April 27, 2010.
48. “First-Principles Simulations of Inorganic Nanowires”, J. W. Mintmire, Sanibel Symposium, Saint Simons Island, GA, March 1, 2010.
47. “First-Principles Simulations of Graphitic Nanoribbons”, J. W. Mintmire, J. W. Li, D. Gunlycke, and C. T. White, 2009 Fall ACS National Meeting, Washington, DC, August 17, 2009.
46. “Optoelectronic Properties of Carbon Nanostructures”, J. W. Mintmire, 2009 DOE EPSCoR Annual Program Review and Workshop, Long Island, NY, July 21, 2009.
45. “Computational Tools for Nanostructure Simulations”, J. W. Mintmire and T. Jayasekera, 3rd Canadian Conference on Nonlinear Solid Mechanics (CanCNSM2008), Toronto, ON, Canada, June 27, 2008.
44. “Large-Scale Calculations of Quasi-One-Dimensional Nanostructures”, J. W. Mintmire, Workshop on Multiscale and Large-Scale Simulations in DoD Materials Science, MITRE Corporation, McLean, VA, June 15, 2007.
43. “Computational Modeling of Quasi-One-Dimensional Nanostructures”, J. W. Mintmire, International Conference on Nanoscience and Technology, China 2007 (ChinaNANO 2007), Beijing, China, June 4, 2007.
42. “Computational Modeling of Quasi-One-Dimensional Nanostructures,” J. W. Mintmire, Oklahoma EPSCoR Annual State Conference, University of Oklahoma, Norman, OK, May 18, 2006.
41. “Chiral Dependent Optical Properties of Carbon Nanotubes”, J. W. Mintmire, 2005 American Physical Society March National Meeting, Los Angeles, CA, March 21, 2005. [Bull. Am. Phys. Soc. **50**, 199 (2005)].
40. “Computational Tools for Helical Nanostructures”, J. W. Mintmire and C. T. White, 2004 Materials Research Society Fall Meeting, Boston, MA, December 2, 2004.
39. “Computational Simulations of Nanotubes and Nanowires”, J. W. Mintmire, XXI Southwest Theoretical Chemistry Conference, Galveston, TX, October 23, 2004.
38. “Computational Models for Nanotubes and Nanowires”, J. W. Mintmire, American Chemical Society Midwest Regional Meeting, Manhattan, KS, October 21, 2004.
37. “First-Principles Methods for Carbon Nanotubes and Other Nanowire Structures”, J. W. Mintmire and C. T. White, XIII National Conference of the Mexican Society for Surface and Vacuum Science, Huatulco, Oaxaca, Mexico, October 1, 2003.

36. “Band Structure with a Twist: Electronic Properties of Carbon Nanotubes”, J. W. Mintmire and C. T. White, International Congress on the Applications of Density Functional Theory in Chemistry and Physics, Brussels, Belgium, September 9, 2003.
35. “Effects of Curvature on the Bandgaps of Quasimetallic Carbon Nanotubes”, C. T. White, J. W. Mintmire, and I. Cabria, Materials Research Society Spring Meeting, San Francisco, CA, April 23, 2003.
34. “Predicting Properties of Carbon Nanotubes: Nanowires with a Twist”, C. T. White and J. W. Mintmire, American Chemical Society National Meeting, New Orleans, LA, March 23, 2003.
33. “A Twisted Tale of Carbon Nanotubes: Electronic Properties Near the Fermi Level”, J. W. Mintmire and C. T. White, Sanibel Symposium, Saint Augustine, FL, February 23, 2003.
32. “Computational Tools for Materials Physics Modeling”, J. W. Mintmire, Nebraska State EPSCoR Conference, Lincoln, NE, April 4, 2002.
31. “Carbon Nanotubes: A New Twist in Materials Physics”, J. W. Mintmire, High School Physics Teachers’ Day Tutorial, 2001 American Physical Society Meeting, Seattle, WA, March 13, 2001.
30. “Electron Transport Properties of Carbon Nanotubes”, J. W. Mintmire and C. T. White, IEEE International Vacuum Electron Sources Conference, Orlando, FL, July 10-13, 2000.
29. “Density Functional Theory Applied to Carbon Nanostructures”, J. W. Mintmire and C. T. White, Conference on Density Functional Theory & DFT Applications to Materials, Antwerp, Belgium, June 8-10, 2000.
28. “Materials by Design for Low-Dimensional Materials”, J. W. Mintmire and C. T. White, DOE Workshop on Computational Materials Science Networks, Saint Augustine, FL, February 25-26, 2000.
27. “Carbon Nanotubes: Band Structure with a Twist”, J. W. Mintmire and C. T. White, Third Congress of the International Society for Theoretical Chemical Physics, (III-CISTCP), UNAM, Mexico City, Mexico, November 13, 1999.
26. “Band Structure Studies of Nanotubes”, J. W. Mintmire, 1998 March American Physical Society Meeting, Los Angeles, CA, March 17, 1998. [Bull. Am. Phys. Soc. **43**, 379 (1998)].
25. “Atomic-Scale Simulations of Low-Dimensional Materials”, J. W. Mintmire, R.A. Jishi, and C. T. White, International Symposium on Novel Materials, Puri, India, March 6, 1997.
24. “Atomistic Simulations of Shock Induced Pore Collapse in Model Materials”, J. W. Mintmire, J.J.C. Barrett, D. H. Robertson and C. T. White, International Conference on Shock Waves in Condensed Matter, Saint Petersburg, Russia, September 5, 1996.
23. “Electronic and Structural Properties of Carbon Nanotubes”, J. W. Mintmire and C. T. White, Second International Congress of the International Society of Theoretical Chemical Physics, New Orleans, LA, April 10, 1996.

22. "Atomic-Scale Simulations of Adhesion and Tribology at Metal-Metal Oxide Interfaces", J. W. Mintmire, Symposium on Parallel Computing in Quantum Chemistry: Developments, Needs and Scope, Maui High Performance Computing Center, Kihei, Maui, HI, December 15, 1995.
21. "Adhesion at Metal-Oxide Interfaces: An Electrostatics Based Model", J. W. Mintmire and F. H. Streitz, International Congress on Adhesion Science and Technology, Amsterdam, Netherlands, October 17, 1995.
20. "Probing Detonations with Molecular Dynamics", C. T. White, J. J. C. Barrett, J. W. Mintmire and D. H. Robertson, International Workshop on New Methods and Numerical Codes for Shock-Wave Processes in Condensed Media, St. Petersburg, Russia, October 10, 1995.
19. "Atomic Scale Simulations of Carbon Nanotubes", C. T. White and J. W. Mintmire, 1995 International Union of Materials Research Societies 4th International Conference on Advanced Materials, Cancun, Mexico, August 27-September 1, 1995.
18. "Atomic-Scale Simulations of Metal-Oxide Adhesion: A Model for Rolling Friction", J. W. Mintmire, Workshop on Physical and Chemical Mechanisms in Tribology, Bar Harbor, ME, August 28, 1995.
17. "Molecular Dynamics Simulations of Detonations", J. W. Mintmire, D. H. Robertson, J.J.C. Barrett and C. T. White, 10th Symposium on Chemical Problems Connected with the Stability of Explosives (Swedish Section for Detonics and Combustion of the Royal Swedish Academy of Sciences). Margretetorp, Sweden, May 31, 1995.
16. "Predicting Properties of Fullerenes and Their Relatives", C. T. White, D. H. Robertson, and J. W. Mintmire, International Workshop on Clusters and Nanostructured Materials, Puri, India, December 29, 1994-January 4, 1995.
15. "Structural Properties of Fullerene Nanotubules", J. W. Mintmire and C. T. White, ACS National Meeting, Washington, DC, August 25, 1994.
14. "Atomistic Simulations of Shock-Induced Chemistry in Solids", C. T. White, J. W. Mintmire, D. W. Brenner and D. H. Robertson, ACS National Meeting, Washington, DC, August 21, 1994.
13. "Molecular Dynamics Simulations of Detonations", C. T. White, D. H. Robertson, D. W. Brenner and J. W. Mintmire, International Conference on Shock Waves in Condensed Matter, St. Petersburg, Russia, July 18-22, 1994.
12. "First-Principles of Fullerene Tubules", J. W. Mintmire, D. H. Robertson, and C. T. White, 1994 Electrochemical Society National Meeting, San Francisco, CA, May, 1994.
11. "Properties of Graphitic Tubules", B. I. Dunlap, J. W. Mintmire, D. H. Robertson, D. W. Brenner and C. T. White, Spring 1993 Electrochemical Society Meeting, New Orleans, LA, October 10-15, 1993.
10. "Electronic and Structural Properties of Fullerene Tubules", J. W. Mintmire, New York State Section APS Symposium on Nanostructures, Buffalo, NY, October 22, 1993.
9. "Electronic and Structural Properties of Fullerene Tubules", J. W. Mintmire, US-Japan Seminar on Chemistry and Physics of C₆₀ and Related Compounds, Honolulu, HI, July 23, 1993.

8. "Molecular Dynamics Simulations of Void Collapse Mechanisms in Shocked Media", J.W. Mintmire, AIRAPT/APS High Pressure Science and Technology Conference, Colorado Springs, CO, June 30, 1993 [*Bull. Am. Phys. Soc.* **38**, 1524 (1993)].
7. "Helical and Structural Properties of Graphitic Tubules", D. H. Robertson, B. I. Dunlap, D. W. Brenner, J. W. Mintmire and C. T. White, MRS National Meeting, San Francisco, CA, April 12, 1993.
6. "LDF Electronic Structure of Helical Chain Polymers", J. W. Mintmire, Sanibel Symposia, St. Augustine, FL, March 19, 1993.
5. "Electronic and Structural Properties of Fullerene Tubules", J. W. Mintmire, D. H. Robertson, D. W. Brenner, B. I. Dunlap, R. C. Mowrey and C. T. White, MRS National Meeting, Boston, MA, November 30, 1992.
4. "Simulations of Condensed Phase Detonations", C. T. White, D. H. Robertson, D. W. Brenner, J. W. Mintmire and M. L. Elert, DRET and ONR Europe Workshop on Understanding Detonations at the Molecular Level, Paris, France, June 7, 1991.
3. "First-Principles Studies of Polysilane Model Systems", J. W. Mintmire and J. V. Ortiz, American Chemical Society Annual Meeting, Washington, DC, August 26-30, 1990.
2. "Polymer Band Structure Calculations in the Framework of the Density Functional Theory", J. W. Mintmire, Third SCF Users Group Meeting, Facultes Universitaires Notre-Dame de Paix, Namur, Belgium, June 11, 1990.
1. "LDA Geometry Optimization of Polymers", J. W. Mintmire, Ohio Supercomputer Center Workshop on Theory and Applications of Density Functional Approaches to Chemistry, Columbus, OH, May 8, 1990.

Contributed Talks at Professional Society Meetings:

113. "A Twist on Graphene Nanoribbons", J. W. Li, J. W. Mintmire, D. Gunlycke, and C. T. White, 2010 March American Physical Society Meeting, Portland, OR, March 17, 2010.
112. "Electron Transport in Fluorinated Single Wall Nanotubes", T. Jayasekera, J. W. Li, J. W. Mintmire, and V. Meunier, 2009 March American Physical Society Meeting, Pittsburgh, PA, March 16, 2009.
111. "First-Principles Simulations of Silicon Nanowires with Different Surface Passivations", J.W. Li and J. W. Mintmire, 2009 March American Physical Society Meeting, Pittsburgh, PA, March 17, 2009.
110. "Effect of Phase-Breaking Events on Electron Transport in Single-Wall Nanotubes", T. Jayasekera, P. Pillalamarri, and J. W. Mintmire, 2008 March American Physical Society Meeting, New Orleans, LA, March 12, 2008.
109. "Binary Memory Switching in Zigzag-Edge Graphene Nanostrips", D. Gunlycke, D. A. Areshkin, J. W. Mintmire, J. W. Li, and C. T. White, 2008 March American Physical Society Meeting, New Orleans, LA, March 11, 2008.
108. "Band Gaps in Armchair-Edge Graphene Nanostrips", C. T. White, D. Gunlycke, and J.W. Mintmire, 2008 March American Physical Society Meeting, New Orleans, LA, March 10, 2008.

107. “First-Principles Calculations of Zigzag-Edge Graphene Nanostrips with Different Edge Species”, J. W. Mintmire, D. Gunlycke, J. W. Li, and C. T. White, 2008 March American Physical Society Meeting, New Orleans, LA, March 10, 2008.
106. “First-Principles Helical Elasticity in Carbon Nanotubes”, H. M. Lawler, J. W. Mintmire, D. A. Areshkin, D. Gunlycke, and C. T. White, 2007 March American Physical Society Meeting, Denver, CO, March 7, 2007.
105. “Applications of Nanoribbon Devices”, T. Jayasekera and J. W. Mintmire, 2007 March American Physical Society Meeting, Denver, CO, March 7, 2007.
104. “First-Principles Simulations of Armchair-Edge Graphene Nanostrips”, J. Li, J. W. Mintmire, D. Gunlycke, and C. T. White, 2007 March American Physical Society Meeting, Denver, CO, March 7, 2007.
103. “Spin-Polarized States in Zigzag-Edge Graphene Nanostrips”, J. W. Mintmire, J. Li, D. Gunlycke, and C. T. White, 2007 March American Physical Society Meeting, Denver, CO, March 6, 2007.
102. “Ab initio Study of the Electronic Structures and Optical Properties of ZnO Single-Wall Nanotubes”, S. L. Elizondo and J. W. Mintmire, 2006 Materials Research Society Fall Meeting, November 29, 2006.
101. “First-Principles Electronic Properties of Graphene Nanostrips”, J. W. Mintmire, Junwen Li, and C. T. White, 2006 Materials Research Society Fall Meeting, November 28, 2006.
100. “First-Principles Optical Cross-Sections of Ultrathin ZnO Nanowires”, S. L. Elizondo, J. W. Mintmire, 2006 March American Physical Society Meeting, Baltimore, MD, March 16, 2006.
99. “First Principles Properties of Polymeric Photovoltaic Materials”, T. Jayasekera, J. W. Mintmire, 2006 March American Physical Society Meeting, Baltimore, MD, March 15, 2006.
98. “Ballistic Conductance in Narrow Graphene Strips”, D. Areshkin, J. W. Mintmire, C. T. White, 2006 March American Physical Society Meeting, Baltimore, MD, March 15, 2006.
97. “Calculation of the Vibrational Continuum in Helical Polymers from First Principles: Application to Single-Walled Carbon Nanotubes”, H. Lawler, C. T. White, J. W. Mintmire, 2006 March American Physical Society Meeting, Baltimore, MD, March 14, 2006.
96. “Ab Initio Study of Helical Silver Single-Wall Nanotubes and Nanowires”, S. L. Elizondo and J. W. Mintmire, 2005 Materials Research Society Fall Meeting, Boston, MA, December 1, 2005.
95. “Diameter Dependence of the Radial-Breathing Frequency in Carbon Nanotubes and Its Relation to Properties of Bulk Graphite”, H. Lawler, C. T. White, and J. W. Mintmire, 2005 Materials Research Society Fall Meeting, Boston, MA, November 30, 2005.
94. “First-Principles Optoelectronic Properties of Potential Organic Polymer Photovoltaic Materials”, T. Jayasekera, S. L. Elizondo, and J. W. Mintmire, 2005 Materials Research Society Fall Meeting, Boston, MA, November 29, 2005.

93. “First-Principles Optical Cross-Sections for Single-Walled Carbon Nanotubes”, S. Nandi, S. L. Elizondo, and J. W. Mintmire, 2004 Materials Research Society Fall Meeting, Boston, MA, December 1, 2004.
92. “Density Functional Simulation of Metallic Carbon Nanowires”, R. K. Vadapalli and J.W. Mintmire, American Chemical Society Midwest Regional Meeting, Manhattan, KS, October 21, 2004.
91. “First-Principles Optical Cross-Sections for Single-Walled Carbon Nanotubes”, S.L. Elizondo, S. Nandi, and J. W. Mintmire, American Chemical Society Midwest Regional Meeting, Manhattan, KS, October 21, 2004.
90. “First-Principles Treatment of van Hove Singularity Dependence on Nanotube Conformation”, I. Cabria, C. T. White, and J. W. Mintmire, 2004 American Physical Society Meeting, Montreal, Quebec, Canada, March 26, 2004.
89. “Comparative Study of One-Electron Effects on the Density of States of Single-Wall Carbon Nanotubes”, C. T. White, I. Cabria, and J. W. Mintmire, 2004 American Physical Society Meeting, Montreal, Quebec, Canada, March 24, 2004.
88. “Stability and Electronic Structure of Black-Phosphorus Nanotubes”, I. Cabria and J. W. Mintmire, 2003 American Physical Society Meeting, Austin, TX, March 7, 2003. [Bull. Am. Phys. Soc. **48**, 1329 (2003)]
87. “First-Principles Properties of Narrow Carbon Nanotubes”, J. W. Mintmire, I. Cabria, and C. T. White, 2003 American Physical Society Meeting, Austin, TX, March 3, 2003. [Bull. Am. Phys. Soc. **48**, 303 (2003)]
86. “An Object-Oriented Framework for Parallel, Reactive Molecular Dynamics Simulations”, S. J. Stuart, Y. Li, and J. W. Mintmire, IASTED International Conference on Parallel and Distributed Computing and Systems (PDCS 2002), Cambridge, MA, November 6, 2002.
85. “The Largest Band Gap Carbon Nanotubes”, I. Cabria, J. W. Mintmire, and C. T. White, 2002 American Physical Society Meeting, Indianapolis, IN, March 19, 2002.
84. “Quasimetallic Carbon Nanotube Band Gaps”, C. T. White, I. Cabria, and J. W. Mintmire, 2002 American Physical Society Meeting, Indianapolis, IN, March 19, 2002.
83. “Effects of Fluorination on Single-Wall Carbon Nanotubes”, N. C. Braier, R. A. Jishi, J.W. Mintmire, and C. T. White, 2001 American Physical Society Meeting, Seattle, WA, March 16, 2001. [Bull. Am. Phys. Soc. **46**, 1166 (2001)]
82. “Electronic Structure of Narrow Carbon Nanotubes”, J. W. Mintmire, N. C. Braier, and C. T. White, 2001 American Physical Society Meeting, Seattle, WA, March 13, 2001. [Bull. Am. Phys. Soc. **46**, 498 (2001)]
81. “Band Structure Effects on Electron Transport in DNA”, R. A. Jishi, J. Bragin, J. W. Mintmire, and C. T. White, 2001 American Physical Society Meeting, Seattle, WA, March 12, 2001. [Bull. Am. Phys. Soc. **46**, 89 (2001)].
80. “Surface Reconstruction of Alumina Surfaces”, J. W. Mintmire, International Conference on Metallurgical Coatings and Thin Films (ICMCTF), San Diego, CA, April 10, 2000.
79. “Universal Density of States of Carbon Nanotubes”, J. W. Mintmire and C. T. White, 1999 March American Physical Society Meeting, Atlanta, GA, March 25, 1999 [Bull. Am. Phys. Soc. **44**, 1652 (1999)].

78. “Molecular Dynamics Simulations of Nanotribology in Ceramics”, D. J. Keffer and J. W. Mintmire, 1998 March American Physical Society Meeting, Los Angeles, CA, March 19, 1998. [*Bull. Am. Phys. Soc.* **43**, 852 (1998)].
77. “Energetics of Vacancy Occupation in gamma-Alumina”, F. H. Streitz and J. W. Mintmire, 1998 March American Physical Society Meeting, Los Angeles, CA, March 18, 1998. [*Bull. Am. Phys. Soc.* **43**, 626 (1998)].
76. “Detonation Hugoniot from Molecular Dynamics Simulations”, D. R. Swanson, J. W. Mintmire, M. L. Elert, and D. H. Robertson, 1998 March American Physical Society Meeting, Los Angeles, CA, March 17, 1998. [*Bull. Am. Phys. Soc.* **43**, 406 (1998)].
75. “Effect of Layer-Layer Interaction on BN Nanotubes”, C. T. White, J. W. Mintmire, and R. A. Jishi, 1998 March American Physical Society Meeting, Los Angeles, CA, March 17, 1998. [*Bull. Am. Phys. Soc.* **43**, 380 (1998)].
74. “Electronic Properties of Peptide Nanotubes”, R. A. Jishi, J. Bragin, N. C. Braier, J. W. Mintmire, and C. T. White, 1998 March American Physical Society Meeting, Los Angeles, CA, March 17, 1998. [*Bull. Am. Phys. Soc.* **43**, 379 (1998)].
73. “Energetics of cation vacancy occupation in γ -alumina,” F. H. Streitz and J. W. Mintmire, Annual Meeting of The Minerals, Metals and Materials Society, San Antonio, TX, February 16-20, 1998.
72. “Molecular Dynamics Simulations of Friction at the Interfaces of Electrostatic Materials”, D. J. Keffer and J. W. Mintmire, AIChE Annual Meeting, Los Angeles, CA, November 16-21, 1997.
71. “First-Principles Simulations of Endohedral Selenium in Nanotubes”, R. A. Jishi, J. W. Mintmire and C. T. White, APS National Meeting, Kansas City, MO, March 17, 1997 [*Bull. Am. Phys. Soc.* **42**, 46 (1997)].
70. “Atomic-Scale Simulations of Nanoindentation and Friction in Ceramics”, D. J. Keffer and J. W. Mintmire, APS National Meeting, Kansas City, MO, March 17, 1997 [*Bull. Am. Phys. Soc.* **42**, 46 (1997)].
69. “Cation Vacancy Occupation in α -Alumina”, F. H. Streitz and J. W. Mintmire, MRS National Meeting, Boston, MA, December 3, 1996.
68. “Atomic-Scale Simulations of Structural Properties of Ceramics”, J. W. Mintmire and F.H. Streitz, MRS National Meeting, Boston, MA, December 3, 1996.
67. “Atomic Scale Simulations of Adhesion and Tribology at Metal-Metal Oxide Interfaces”, J. W. Mintmire and F. H. Streitz, MRS National Meeting, Boston, MA, November 30, 1995.
66. “Effects on Nanotube Voids on the Sensitivity of Model Energetic Materials”, C. T. White, J. J. C. Barrett and J. W. Mintmire, MRS National Meeting, Boston, MA, November 29, 1995.
65. “Optical Properties of Carbon Nanotubes”, J. W. Mintmire and C. T. White, MRS National Meeting, Boston, MA, November 27, 1995.
64. “Electronic Structure Simulations of Carbon Nanotubes”, J. W. Mintmire and C. T. White, EMRS 1995 Spring Meeting, Strasbourg, France, May, 25, 1995.
63. “Model Simulations of Shear and Tensile Strain of Metal-Oxide Interfaces”, J. W. Mintmire and F. H. Streitz, APS National Meeting, San Jose, CA, March 21, 1995. [*Bull. Am. Phys. Soc.* **40**, 282 (1995)].

62. "Atomic Scale Simulations of Metal-Oxide Interfaces", F. H. Streitz and J. W. Mintmire, APS National Meeting, San Jose, CA, March 21, 1995. [*Bull. Am. Phys. Soc.* **40**, 242 (1995)].
61. "Adhesion at Metal-Ceramic Interfaces: An Electrostatics-Based Model", J. W. Mintmire and F. H. Streitz, Adhesion Society Annual Meeting, Hilton Head, SC, February 20, 1995.
60. "Atomic-Scale Simulation of Aluminum-Alumina Interfaces", F. H. Streitz and J. W. Mintmire, MRS National Meeting, Boston, MA, November 30, 1994.
59. "First-Principles Electronic Structure Simulations of Carbon Nanotubes", J. W. Mintmire and C. T. White, MRS National Meeting, Boston, MA, November 29, 1994.
58. "Structural Properties of Metal-Oxide Interfaces", J. W. Mintmire and F. H. Streitz, Southeast Section APS Regional Meeting, Newport News, VA, November 10, 1994.
57. "Molecular Dynamics Simulations of Metal-Oxide Surfaces and Interfaces", F. H. Streitz and J. W. Mintmire, AVS National Meeting, Denver, CO, October 25, 1994.
56. "Electrostatic Potentials for Metal-Oxide Surfaces and Interfaces", F. H. Streitz and J. W. Mintmire, Fifth International Conference on Composite Interfaces, Gothenberg, Sweden, June 20, 1994.
55. "Molecular Dynamics with Charge Transfer at Metal-Oxide Interfaces", F. H. Streitz and J. W. Mintmire, 1994 International Conference on Metallurgical Coatings and Thin Films, San Diego, CA, April 25, 1994.
54. "Structural Properties of Fullerene Nanotubules", J. W. Mintmire and C. T. White, APS National Meeting, Pittsburgh, PA, March 24, 1994 [*Bull. Am. Phys. Soc.* **39**, 820 (1994)].
53. "Structural Properties of Metal-Oxide Interfaces", F. H. Streitz and J. W. Mintmire, APS National Meeting, Pittsburgh, PA, March 24, 1994 [*Bull. Am. Phys. Soc.* **39**, 820 (1994)].
52. "Charge Transfer at Transition-Metal Oxide Interfaces", F. H. Streitz and J. W. Mintmire, MRS National Meeting, Boston, MA, December 3, 1993.
51. "Electronic and Structural Properties of Fullerene Nanotubules", J. W. Mintmire and C.T. White, MRS National Meeting, Boston, MA, December 2, 1993.
50. "Charge Transfer at Transition Metal Oxide Interfaces", F. H. Streitz and J. W. Mintmire, APS National Meeting, Seattle, WA, March 24, 1993.
49. "Helical and Rotational Symmetries and Bandgaps of Graphitic Tubules", J. W. Mintmire and C. T. White, APS National Meeting, Seattle, WA, March 22, 1993.
48. "Theoretical Study of Surface-Defect Luminescence from Hydrogenated Silicon Clusters", A.H. Edwards, D. Babic, R. Tsu, J. W. Mintmire, and C. T. White, MRS National Meeting, Boston, MA, December 2, 1992.
47. "Molecular Simulations of Shock-Induced Chemistry in Energetic Materials", C. T. White, D. H. Robertson, M. L. Elert, J. W. Mintmire and D. W. Brenner, MRS National Meeting, Boston, MA, December 1, 1992.
46. "Electronic Properties of Model Silicon-Based Quantum Wires", J. W. Mintmire, AVS National Meeting, Chicago, IL, November 10, 1992.

45. “Many-Body Effects in STM of Molecular Adsorbates”, J. W. Mintmire, J. A. Harrison, R. J. Colton, and C. T. White, IVC-12/ICSS-8, The Hague, Netherlands, October 13, 1992.
44. “Theory for New Carbon-Based Structures”, D. W. Brenner, B. I. Dunlap, R. C. Mowrey, J. W. Mintmire, J. A. Harrison, D. H. Robertson, M. Lyons and C. T. White, MRS National Meeting, San Francisco, CA, April 27-May 1, 1992.
43. “Electronic Structure of Fullerene Tubules”, J. W. Mintmire, D. H. Robertson, B. I. Dunlap and C. T. White, APS National Meeting, Indianapolis, IN, March 20, 1992 [*Bull. Am. Phys. Soc.* **37**, 795 (1992)].
42. “First-Principles Torsional Potentials of Organopolysilanes”, J. W. Mintmire, APS National Meeting, Indianapolis, IN, March 18, 1992 [*Bull. Am. Phys. Soc.* **37**, 498 (1991)].
41. “Photoelectron Spectra of $C_{60}H_{36}$ and $C_{60}H_{60}$ ”, B. I. Dunlap, J. W. Mintmire, D. H. Robertson, D. W. Brenner, R. C. Mowrey and C. T. White, MRS National Meeting, Boston, MA, December 5, 1991.
40. “Electronic Structure of Fullerene Tubules”, J. W. Mintmire, D. H. Robertson, B. I. Dunlap, R. C. Mowrey, D. W. Brenner and C. T. White, MRS National Meeting, Boston, MA, December 5, 1991.
39. “Many-Body Effects in Scanning-Tunneling Microscopy of Molecular Adsorbates”, J.W. Mintmire, J.A. Harrison, R.J. Colton and C. T. White, AVS National Meeting, Seattle, WA, November 13, 1991.
38. “Molecular Dynamics Simulations of Void and Defect Effects on Shock Waves in Solid Media”, J. W. Mintmire, D. H. Robertson, D. W. Brenner and C. T. White, APS Topical Conference on Shock Compression of Condensed Matter, Williamsburg, VA, June 18, 1991 [*Bull. Am. Phys. Soc.* **36**, 1832 (1991)].
37. “Local-Density Approach to Helical Chain Polymers”, J. W. Mintmire, APS National Meeting, Cincinnati, OH, March 20, 1991 [*Bull. Am. Phys. Soc.* **36**, 800 (1991)].
36. “First-Principles Study of Radical Addition to Diamond {111} Surfaces”, C. T. White, J.W. Mintmire, D. W. Brenner, B. I. Dunlap and R. C. Mowrey, APS National Meeting, Cincinnati, OH, March 20, 1991 [*Bull. Am. Phys. Soc.* **36**, 778 (1991)].
35. “Geometric and Electric Structures of $C_{60}H_{60}$, $C_{60}F_{60}$, and $C_{60}H_{36}$ ”, B. I. Dunlap, D. W. Brenner, J. W. Mintmire, R. C. Mowrey, D. H. Robertson and C. T. White, APS National Meeting, Cincinnati, OH, March 18, 1991.
34. “Local Density Functional Photoelectron Spectra of Selected Fullerenes”, J. W. Mintmire, B. I. Dunlap, D. W. Brenner, R. C. Mowrey and C. T. White, APS National Meeting, Cincinnati, OH, March 18, 1991.
33. “Simulations of C_{60} with Diamond Surfaces”, R. C. Mowrey, J. W. Mintmire, D. W. Brenner, B. I. Dunlap and C. T. White, APS National Meeting, Cincinnati, OH, March 18, 1991 [*Bull. Am. Phys. Soc.* **36**, 353 (1991)].
32. “Molecular Dynamics Simulations of Collisions of Buckminsterfullerene with Diamond Surfaces”, R. C. Mowrey, D. W. Brenner, B. I. Dunlap, J. W. Mintmire and C. T. White, MRS National Meeting, Boston MA, November 29, 1990.

31. "First-Principles Study of Soliton Hyperfine Interactions in Polyacetylene", C. T. White, F. W. Kutzler, J. W. Mintmire and M. R. Cook, MRS National Meeting, Boston, MA, November 29, 1990.
30. "Possible Structures of $C_{60}H_{36}$ ", B. I. Dunlap, D. W. Brenner, R. C. Mowrey, J. W. Mintmire, D. H. Robertson and C. T. White, MRS National Meeting, Boston, MA, November 28, 1990.
29. "First-Principles Study of Photoexcited Defects in Polysilane Chains", J. W. Mintmire, R.C. Mowrey, D. W. Brenner, B. I. Dunlap and C. T. White, MRS National Meeting, Boston, MA, November 28, 1990.
28. "Molecular-Dynamics Simulations of the Reaction of Atomic Hydrogen with Diamond Surfaces", D. W. Brenner, B. I. Dunlap, J. W. Mintmire, R. C. Mowrey and C. T. White, Second International Conference on the New Diamond Science and Technology, Washington, DC, September 25, 1990.
27. "First-Principles Simulations of Diamond Surface Formation Via Radical Addition", J.W. Mintmire, D. W. Brenner, B. I. Dunlap, R. C. Mowrey and C. T. White, Second International Conference on the New Diamond Science and Technology, Washington, DC, September 24, 1990.
26. "Ground State and Vertical Ionization versus Si-Si-Si and C-C-C Bond Angles in Si_3H_8 and C_3H_8 ", J. V. Ortiz and J. W. Mintmire, ACS National Meeting, Washington, DC, August 28, 1990.
25. "Embedded-Atom Method Study of the Supermodulus Effect in Composition-Modulated Superlattices", R.S. Jones and J. W. Mintmire, APS National Meeting, Anaheim, CA, March 16, 1990 [*Bull. Amer. Phys. Soc.* **35**, 780 (1990)].
24. "LDA Antiferromagnetic Ground State of Polyacetylene", J. W. Mintmire and C. T. White, APS National Meeting, Anaheim, CA, March 14, 1990, [*Bull. Amer. Phys. Soc.* **35**, 471 (1990)].
23. "Chemical Forces Associated with Deuterium Confinement in Palladium", B. I. Dunlap, J. W. Mintmire, D. W. Brenner, R. C. Mowrey, H. D. Ladouceur, P. P. Schmidt, C. T. White, and W.E. O'Grady, APS National Meeting, Baltimore, MD, May 2, 1989.
22. "Coherency-Strain in Composition-Modulated Metals", J. W. Mintmire, APS National Meeting, St. Louis, MO, March 20, 1989 [*Bull. Amer. Phys. Soc.* **34**, 492 (1989)].
21. "First-Principles Electronic Structure Calculations of Organopolysilane Materials", J. W. Mintmire, MRS National Meeting, Boston, MA, November 29, 1988.
20. "The Determination of the Structure and Bonding of Polydiacetylene using Local-Density Functional Methods", S.M. Mattar, J. W. Mintmire and C. T. White, Third Chemical Congress of North America, Toronto, Canada, June 8, 1988.
19. "Electronic Structure of Polysilane Model Systems", J. W. Mintmire and J. V. Ortiz, APS National Meeting, New Orleans, LA, March 23, 1988 [*Bull. Amer. Phys. Soc.* **33**, 540 (1988)].
18. "First-Principle Results for the Geometry of cis-Polyacetylene", C. T. White, J. W. Mintmire and M. L. Elert, APS National Meeting, New Orleans, LA, March 22, 1988 [*Bull. Amer. Phys. Soc.* **33**, 457 (1988)].

17. "Density Functional Approach to the Structure of Molecules and Clusters", R.S. Jones and J. W. Mintmire, APS National Meeting, New Orleans, LA, March 21, 1988 [*Bull. Amer. Phys. Soc.* **33**, 278 (1988)].
16. "Electronic Structure Conformation Studies of Polysilane Model Systems", J. W. Mintmire and J. V. Ortiz, ACS Topical Workshop on Advances in Silicon-Based Polymer Science, Makaha, HI, November 22, 1987.
15. "Electronic Properties of Heterocyclic Ring Chain Polymers", J. W. Mintmire and C. T. White, at 39th ACS Southeast Regional Meeting, Orlando, FL, November 5, 1987.
14. "Peierls Dimerization Within the Local-Density Functional Formalism", J. W. Mintmire and C.T. White, at APS National Meeting, New York, NY, March 20, 1987 [*Bull. Amer. Phys. Soc.* **32**, 929 (1987)].
13. "Band Structure of Polysilane Chains", J. W. Mintmire, at APS National Meeting, New York, NY, March 19, 1987 [*Bull. Amer. Phys. Soc.* **32**, 828 (1987)].
12. "Direct Geometry Optimization for Local-Density Functional Methods Using Energy Gradient Techniques", J. W. Mintmire and C. T. White, at APS National Meeting, Las Vegas, NV, April 1, 1986 [*Bull. Amer. Phys. Soc.* **31**, 353 (1986)].
11. "Kinetic Energy Release Accompanying Gas Phase Dissociation of Polynitroaromatics and Nitramines", R. J. Doyle, Jr., J. W. Mintmire and J. E. Campana, at ACS National Meeting, Miami Beach, FL, April 30, 1985.
10. "Electronic Structure of Heterocyclic Ring Chain Polymers", J. W. Mintmire and C. T. White, at 19th MARM Meeting of the ACS, Monmouth College, West Long Branch, NJ, May 21, 1985.
9. "Photoelectron Spectra of Metal Phthalocyanines", F. W. Kutzler, J. W. Mintmire and C.T. White, at APS National Meeting, Baltimore, MD, March 29, 1985 [*Bull. Amer. Phys. Soc.* **30**, 607 (1985)].
8. "Band Structure and Crystal Packing Calculations for Helical Polyacetylene", M. L. Elert, C. T. White and J. W. Mintmire, at APS National Meeting, Baltimore, MD, March 28, 1985 [*Bull. Amer. Phys. Soc.* **30**, 566 (1985)].
7. "First-Principles Calculations of CH_x", C. T. White, F.W. Kutzler and J. W. Mintmire, at APS National Meeting, Baltimore, MD, March 28, 1985 [*Bull. Amer. Phys. Soc.* **30**, 566 (1985)].
6. "Electronic Structure Calculations for Heterocyclic Ring Chain Polymers", J. W. Mintmire, C. T. White and JM. L. Elert, at APS National Meeting, Baltimore, MD, March 27, 1985 [*Bull. Amer. Phys. Soc.* **30**, 471 (1985)].
5. "Local-Density Functional Approach to Chain Polymers", J. W. Mintmire and C. T. White, at 1984 International Chemical Congress of Pacific Basin Societies, Honolulu, HI, December 18, 1984.
4. "Dielectric Response Properties of all *trans*-Polyacetylene", J. W. Mintmire and C. T. White, at APS National Meeting, Los Angeles, CA, March 21, 1983 [*Bull. Amer. Phys. Soc.* **28**, 245 (1983)].
3. "Study of Localization Effects on XVV Auger Lineshapes of Chemisorbed Species", C. T. White, E.N. Economou and J. W. Mintmire, at APS National Meeting, Dallas, TX, March 11, 1982 [*Bull. Amer. Phys. Soc.* **27**, 375 (1982)].

2. “Effects of Disorder on Pople-Walmsley Defects in *trans*-Polyacetylene”, C. T. White, M. L. Elert and J. W. Mintmire, at APS National Meeting, Dallas, TX, March 11, 1982 [*Bull. Amer. Phys. Soc.* **27**, 375 (1982)].
1. “Local Density Functional Calculations on Polyacetylene”, J. W. Mintmire and C. T. White, at APS National Meeting, Dallas, TX, March 10, 1982 [*Bull. Amer. Phys. Soc.* **27**, 313 (1982)].

Contributed Talks at Other Professional Meetings & Workshops

57. “First-Principles Simulations of Inorganic Nanowires”, J. W. Li, T. Jayasekera, and J. W. Mintmire, Sanibel Symposium. Saint Simons Island, GA, February 27, 2009.
56. “Electronic Properties of Quasi-One-Dimensional Nanostructures”, J. W. Mintmire, T. Jayasekera, J. W. Li, P. Pillalamarri, V. Jogireddy, and V. Meunier, 2008 DOE EPSCoR Program Review Workshop, Oak Ridge, TN, July 22-24, 2008.
55. “Effect of Phase-Breaking Events on Electron Transport in Long-Range Mesoscopic and Nano Systems”, T. Jayasekera, P. Pillalamarri, J. W. Mintmire, and V. Meunier, Sanibel Symposium, Saint Simons Island, February 25, 2008.
54. “First-Principles Optoelectronic Properties of Quasi-One-Dimensional Nanostructured Materials”, J. W. Mintmire, T. Jayasekera, and J. W. Li, Sanibel Symposia, Saint Simons Island, GA, February 22, 2008.
53. “Optoelectronic Properties of Carbon Nanostructures”, J. W. Mintmire and T. Jayasekera, 2007 DOE EPSCoR Program Review Workshop, Golden, CO, July 23-25, 2007.
52. “Transport in Graphene Multi-Terminal Devices Effect of Geometry and Lattice Defects”, T. Jayasekera and J. W. Mintmire, Sanibel Symposia, Saint Simons Island, GA, February 26, 2007.
51. “First-Principles Simulations of Graphene Nanostrips”, J. Li, J. W. Mintmire, D. Gunlycke, and C. T. White, Sanibel Symposia, Saint Simons Island, GA, February 26, 2007.
50. “First-Principles Simulations of Nanoscale Devices: Computational Materials Physics at Oklahoma State University”, S. L. Elizondo, T. Jayasekera, and J. W. Mintmire, Oklahoma EPSCoR Annual State Conference, University of Oklahoma, Norman, OK, May 18, 2006.
49. “First-Principles Properties of Organic Polymer Photovoltaic Materials”, T. Jayasekera, S. L. Elizondo, and J. W. Mintmire, International Conference on Chemical Reactivity, Brussels, Belgium, April 5, 2006.
48. “First-Principles Simulations of Chiral Double-Wall Carbon Nanotubes”, B. A. Landis, J.R. Weierman, and J. W. Mintmire, Sanibel Symposia, Saint Simons Island, GA, February 28, 2006.
47. “Endohedral Carbon in Single-Wall Carbon Nanotubes”, R. K. Vadapalli and J. W. Mintmire, Conference in Current Trends in Computational Chemistry 2005, Jackson, MS, November 4-5, 2005.

46. "First-Principles Optical Cross-Sections for Single-Walled Carbon Nanotubes", S. L. Elizondo, S. Nandi, and J. W. Mintmire, Sanibel Symposia, Saint Simons Island, GA, March 8, 2005..
45. "Theoretical Elastic Properties of Single Walled Carbon Nanotubes", J. T. Alford, B. A. Landis, and J. W. Mintmire, Sanibel Symposia, Saint Simons Island, GA, March 8, 2005.
44. "Computational Tools for Nanostructure Simulations", R. K. Vadapalli, B. A. Landis, and J. W. Mintmire, Molecular Quantum Mechanics Conference, Cambridge, England, July 26, 2004.
43. "First-Principles Properties of Narrow Carbon Nanotubes", J. W. Mintmire, I. Cabria, and C. T. White, Sanibel Symposium, Saint Augustine, FL, February 23, 2002.
42. "Computational Materials Science of Low-Dimensional Materials", J. W. Mintmire, ONR Computational Chemical Dynamics Research Workshops, Arlington, VA, October 4, 2001. (invited)
41. "Surface Reconstruction of Alumina Surfaces", J. W. Mintmire, Sanibel Symposium, Saint Augustine, FL, February 24, 2001.
40. "Object-Oriented Molecular Dynamics Software for Energetic and Nonenergetic Materials", J. W. Mintmire, Workshop on Multiscale Modeling of Materials, Newport, RI, May 17-19, 2000.
39. "Cell Multipole Methods within the ES+ Approach", J. W. Mintmire and D. J. Keffer, Sanibel Symposium, Saint Augustine, FL, February 26, 2000.
38. "Ceramic Thin Films and Coating", J. W. Mintmire, NRL Grand Challenge Workshop: Naval Materials by Design", US Naval Research Laboratory, September 27, 1999.
37. "Efficient Parallel Algorithms for Molecular Dynamics Simulations Using Variable Charge Transfer Electrostatic Potentials", J. W. Mintmire, AFOSR/ONR/NSF Tribology Program Review, Islamorada, FL, 17 June 1999. (invited)
36. "Theoretical Predictions: Carbon Nanotubes", C. T. White and J. W. Mintmire, DoD Defense Science & Technology Seminar on Emerging Technologies, Arlington, VA, March 19, 1999. (invited)
35. "Theoretical Simulations of Low-Dimensional Materials", J. W. Mintmire and C. T. White, AFOSR/ONR/NSF Tribology Program Review, Annapolis, MD, 22-25 June 1998. (invited)
34. "Theoretical Simulations of Carbon Nanotubes", J. W. Mintmire, ONR MURI kickoff meeting, UNC-Chapel Hill, NC, May 14, 1998. (invited)
33. "Molecular Dynamics Simulations of Ceramics", J. W. Mintmire, AFOSR/ONR Tribology Program Review, Englewood, OH, June 26, 1997. (invited)
32. "Shock-Induced Collapse of Nanoscale Voids in Molecular Solids", J. W. Mintmire, D.H. Robertson and C. T. White, Shock, Mechanical and Thermal Initiation-to-Detonation Workshop, Los Alamos, NM, November 16-18, 1993.
31. "Atomic Potentials with Charge Transfer for Metal Oxide Systems", F. H. Streitz and J.W. Mintmire, Workshop on the Appraisal of Models for the Atomistic Simulation of Complex Systems, Bad Honnef, Germany, September 26-30, 1993.

30. “Molecular Description of Chemically-Sustained Shock Waves: From Initiation to Continuum Behavior in a Hundred Picoseconds”, C. T. White, D. H. Robertson, J. W. Mintmire, D. W. Brenner and M. L. Elert, TNO-PML/ONR Workshop on Desensitization of Explosives and Propellants, Delft, Netherlands, November 13, 1991. (invited)
29. “Symmetric Charge Transfer Excitations in C_{60} ”, C. T. White, R. C. Mowrey, D. W. Brenner, B. I. Dunlap and P.P. Schmidt, International Symposium on the Physics and Chemistry of Finite Systems: From Clusters to Crystals, Richmond, VA, October 10, 1991.
28. “Relative Energetics of C_{44} Fullerene Isomers”, M. Lyons, B. I. Dunlap, D. W. Brenner, D. H. Robertson, R. C. Mowrey, J. W. Mintmire and C. T. White, International Symposium on the Physics and Chemistry of Finite Systems: From Clusters to Crystals, Richmond, VA, October 10, 1991.
27. “Local Density Functional and Empirical Potential Studies of Fullerene Materials”, B. I. Dunlap, D. W. Brenner, J. W. Mintmire, R. C. Mowrey, C. T. White and P.P. Schmidt, 1991 Gordon Conference on Metal and Semiconductor Clusters, Wolfeboro, NH, August 5-9, 1991.
26. “Geometry Optimization of Molecules Within an LCAO Local-Density Functional Approach”, J. W. Mintmire, Sanibel Symposia, St. Augustine, FL, March 22, 1990.
25. “Model Studies of Helical *cis*-Polyacetylene Oligomers”, C. T. White, M. L. Elert and J.W. Mintmire, Sanibel Symposia, St. Augustine, FL, March 23, 1990.
24. “Limits of Chemical Effects on Cold Fusion”, J. W. Mintmire, B. I. Dunlap, D. W. Brenner, R. C. Mowrey, H. D. Ladouceur, P. P. Schmidt, C. T. White and W. E. O’Grady, LANL Workshop on Cold Fusion Phenomena, Santa Fe, NM, May 23, 1989.
23. “Model Studies of Composition-Modulated Metal Alloys”, J. W. Mintmire, ONR Composite Interfaces Program Review, Leesburg, VA, April 19, 1989.
22. “Geometry Optimization Using Local-Density Functional Methods: Numerical Aspects”, R. S. Jones and J. W. Mintmire, Sanibel Symposia, Marineland, FL, March 18, 1988.
21. “Optical Absorption Properties of Organopolysilane Materials”, J. W. Mintmire, Sanibel Symposia, Marineland, FL, March 14, 1988.
20. “Brillouin Zone Treatment in Total Energy Treatment Calculations of Peierls Distorted Chains”, C. T. White and J. W. Mintmire, Sanibel Symposia, Marineland, FL, March 19, 1987.
19. “Local Density Functional Study of Polysilane Chains”, J. W. Mintmire, Sanibel Symposia, Marineland, FL, March 16, 1987.
18. “Electric Structure of Heterocyclic Ring Chain Polymers”, J. W. Mintmire and C. T. White, International Conference on Science and Technology of Synthetic Metals, Kyoto, Japan, June 2, 1986 [Synth. Metals **19**, 997 (1987)].
17. “Local-Density Functional Spin-Unrestricted Study of Soliton Defects in Polyacetylene”, F.W. Kutzler, C. T. White and J. W. Mintmire, Recent Developments in Polymer Science Symposium, Sandia National Laboratories, Albuquerque, NM, October 16, 1985.

16. "Soliton Defects in Polyacetylene: Local-Density Functional Results", F. W. Kutzler, C.T. White and J. W. Mintmire, Fifth International Congress on Quantum Chemistry, Montreal, Canada, August 19, 1985.
15. "The Metastable Loss of N₂O from Nitramines", R.J. Doyle, Jr., J. W. Mintmire and J.E. Campana, 33rd Annual Conference on Mass Spectrometry and Allied Topics, San Diego, CA, May 30, 1985 [Proc. 33rd Annual Conference of Mass Spectrometry and Allied Topics, 294-295, (1985)].
14. "Theoretical Photoelectron Spectra Using Local-Density Functional Results", J. W. Mintmire, Sanibel Symposia, Marineland, FL, March 21, 1985.
13. "Electronic Structure Calculations on Electroactive Polymers", J. W. Mintmire, Sanibel Symposia, Palm Coast, FL, March 8, 1984.
12. "Spin Magnetic Susceptibility in the Graphite MF₆-Systems", L. Mattix, J. Milliken, H.A. Resing, J. W. Mintmire and M. Rubinstein, 16th Biennial Conference on Carbon, San Diego, Ca, July 1983.
11. "Dielectric Properties of all-trans Polyacetylene", J. W. Mintmire, C. T. White, Sanibel Symposia, Palm Coast, FL, March 11, 1983.
10. "First-Principles Dielectric Function of Polyacetylene", J. W. Mintmire, C. T. White and D.L. Peebles, ICPCCP, Bourg-St.-Maurice, France December 13, 1982.
9. "The Effects of Off-Diagonal Disorder on Soliton-and Polaron-like in Trans-Polyacetylene", C. T. White, M. L. Elert and J. W. Mintmire, ICPCCP, Bourg-St.-Maurice, France, December 13, 1982.
8. "Tight-Binding Studies of Electroactive Organic Polymers", M. L. Elert, J. W. Mintmire and C. T. White, International Conference on the Physics and Chemistry of Conducting Polymers (ICPCCP), Bourg-St.-Maurice, France, December 13, 1982.
7. "Local Density-Functional in Two-Dimensionally Periodic Systems", J. W. Mintmire and J. R. Sabin, Sanibel, Sanibel Symposia, Palm Coast, FL, March 14, 1980.
6. "The F₂ problem Using LCAO-X α ", J. W. Mintmire and J. R. Sabin, SETCA, Tallahassee, FL, May 25, 1979.
5. "Application of the LCAO-X α Method: Studies on CO and F₂", J. W. Mintmire, Sanibel Symposia, Palm Coast, FL, March 13, 1979.
4. "A Study of the Fluorine Molecule Using the LCAO-X α Method", J. W. Mintmire, Sanibel Symposia, Palm Coast, FL, March 22, 1979.
3. "A Comparison of the LCAO-X α and Hartree-Fock Methods on Carbon Monoxide", J.W. Mintmire and J. R. Sabin, Sanibel Symposia, Palm Coast, FL, March 1978.
2. "Interaction of H₂ with Rare Gas Atoms", J. W. Mintmire and J. R. Sabin, Southeast Theoretical Chemist's Association (SETCA) meeting, Tuscaloosa, AL, May 21, 1976.
1. "Ab Initio Studies of Rare Gas Molecules", J. W. Mintmire and J. R. Sabin, Sanibel Symposia, Sanibel, FL, January 1976.

Seminars and Other Oral Presentations

46. "Computational Simulations of Nanostructured Materials", J. W. Mintmire, Department of Physics, Iowa State University, Ames, IA, May 15, 2008.
45. "Computational Simulations of Nanowire and Nanotube Structures", J. W. Mintmire, Physical Chemistry Seminar, Department of Chemistry, Texas Tech University, Lubbock, TX, April 11, 2008. (invited)
44. "Computational Tools for Nanostructure Modeling", J. W. Mintmire, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY, September 18, 2006. (invited)
43. "Computational Modeling of Quasi-One-Dimensional Nanostructures", J. W. Mintmire, Department of Chemistry, University of Tennessee, Knoxville, TN, August 3, 2006. (invited)
42. "Computational Tools for Nanostructure Modeling", J. W. Mintmire, Department of Physics, University of Antwerp, Antwerp, Belgium, April 4, 2006 (invited)
41. "Computational Tools for Nanostructure Modeling", J. W. Mintmire, Department of Chemical, Biological, and Materials Engineering, University of Oklahoma, Norman, OK, January 26, 2006. (invited)
40. "Computational Approaches for Helical Nanostructures", J. W. Mintmire, Oak Ridge National Laboratory, Oak Ridge, TN, June 6, 2005.
39. "First-Principles Excitation Spectra for Single-Walled Carbon Nanotubes", J. W. Mintmire, Third John C. Slater Invited Lecture Series, Quantum Theory Project, University of Florida, Gainesville, FL, October 28, 2004. (invited)
38. "Parallel Algorithms for Computational Modeling of Nanotubes and Nanowires", J. W. Mintmire, Third John C. Slater Invited Lecture Series, Quantum Theory Project, University of Florida, Gainesville, FL, October 27, 2004. (invited)
37. "Computational Tools for Nanostructure Simulations", J. W. Mintmire, Department of Physics, Kansas State University, Manhattan, KS, May 6, 2004. (invited)
36. "First-Principles Methods for Carbon Nanotubes and Other Nanowire Structures", J. W. Mintmire, Center for Nanotechnology Research, NASA Ames Research Center, Moffett Field, CA, November 14, 2003.
35. "Carbon Nanotubes: A New Twist in Materials Physics", J. W. Mintmire, Oak Ridge National Laboratory, Oak Ridge, TN, May 27, 2003. (invited)
34. "Computational Modeling of Nanostructured Materials", Oklahoma EPSCoR NanoNet Seminar Series, Oklahoma State University, Stillwater, OK, February 21, 2003.
33. "Nanoscale Simulations of Metal Oxide Surfaces and Interfaces", J. W. Mintmire, Argonne National Laboratory, Materials Science Division, Argonne, IL, November 4, 2002. (invited)
32. "Carbon Nanotubes: A New Twist in Materials Physics", J. W. Mintmire, Department of Physics, University of Oklahoma, Norman, OK, September 12, 2002 (invited)
31. "Carbon Nanotubes: Band Structure with a Twist", J. W. Mintmire, Department of Physics, University of Texas, Arlington, TX, November 21, 2001. (invited)

30. “Carbon Nanotubes: Band Structure with a Twist”, J. W. Mintmire, Department of Applied Science, College of William & Mary, Williamsburg, VA, October 13, 2000. (invited)
29. “Carbon Nanotubes: Band Structure with a Twist”, J. W. Mintmire, Institute for Theory and Computation in Molecular and Materials Sciences & Department of Physics, University of Florida, Gainesville, FL, July 11, 2000.
28. “Carbon Nanotubes: Band Structure with a Twist”, J. W. Mintmire, Computer Design of Materials Group, Institute for Computational Sciences and Informatics, George Mason University, Fairfax City, VA, November 1, 1999. (invited)
27. “Band Structure of Carbon Nanotubes”, J. W. Mintmire, NIST, Gaithersburg, MD, April 24, 1998. (invited)
26. “Atomic-Scale Simulations of Nanotribology in Ceramics”, J. W. Mintmire, Department of Chemistry, Kansas State University, Manhattan, KS, March 21, 1997. (invited)
25. “Distribution of Cation Vacancy Occupation in γ -alumina,” F. H. Streitz and J. W. Mintmire, Computational Workshop, Vanderbilt University, Nashville, TN, November 5, 1997.
24. “Computational Materials Chemistry: Frontiers at the Nanoscale”, J. W. Mintmire, Department of Chemistry, Indian Institute of Technology, Bombay, India, March 10, 1997. (invited)
23. “Atomic Scale Simulations of Nanotribology in Ceramics”, J. W. Mintmire, Materials Department, Oxford University, Oxford, England, February 28, 1997.
22. “Atomic-Scale Simulations in Materials Chemistry”, J. W. Mintmire, Materials Science & Engineering Department, North Carolina State University, Raleigh, NC, November 15, 1996. (invited)
21. “Atomic Scale Simulations in Materials Chemistry”, J. W. Mintmire, Department of Chemistry, University of New Mexico, NM, October 28, 1994. (invited)
20. “Atomic Scale Simulations at NRL”, J. W. Mintmire, Department of Physics, University of Antwerp-RUCA, Antwerp, Belgium, June 27, 1994.
19. “Atomic Scale Simulations at NRL”, J. W. Mintmire, Department of Chemistry, Odense University, Odense, Denmark, June 24, 1994.
18. “First-Principles of Fullerene Tubules”, J. W. Mintmire, Center for Atomic-scale Materials Physics, Danish Technical University, Lyngby, Denmark, June 22, 1994.
17. “Structural Properties of Fullerene Nanotubules”, J. W. Mintmire, University of California, Irvine, CA, April 29, 1994.
16. “Electronic and Structural Properties of Fullerene Tubules”, J. W. Mintmire, Department of Physics, Virginia Commonwealth University, Richmond, VA November 6, 1992. (invited)
15. “Electronic Properties of Fullerenes”, J. W. Mintmire, Molecular Biophysics Project, Deutsches Krebsforschungszentrum, Heidelberg, Germany, October 19, 1992. (invited)
14. “Electronic Properties of Fullerenes”, J. W. Mintmire, Department of Chemistry, University of New Mexico, Albuquerque, NM, November 15, 1991. (invited)

13. “LDF Electronic Functional Structure of Helical Chain Polymers”, J. W. Mintmire, Technical University of Munich, Garching, Germany, August 12, 1991. (invited)
12. “Optical Properties on Organopolysilanes”, J. W. Mintmire, Department of Chemistry, Georgetown University, Washington, DC, June 21, 1989. (invited)
11. “Electronic Properties of Polysilane Materials”, J. W. Mintmire, Department of Physics, Ohio State University, Columbus, Ohio, December 9, 1988.
10. “LCAO Local-Density Functional Methods for the Total Energies and Electronic Properties of Chain Polymers”, J. W. Mintmire, Department of Chemistry, University of New Brunswick, Fredericton, New Brunswick, Canada, January 8, 1987. (invited)
9. “LCAO Local-Density Functional Methods for the Total Energies of Chain Polymers”, J.W. Mintmire, Department of Physics, University of Texas, Arlington, Texas, September 17, 1986. (invited)
8. “Heteroatom Effects in Heterocyclic Ring Chain Polymers”, J. W. Mintmire, Department of Chemistry, University of New Mexico, Albuquerque, NM, November 2, 1984. (invited)
7. “Local-Density-Functional Approach to all-trans Polyacetylene”, J. W. Mintmire and C.T. White, NRL Chemistry Division Publication Award Presentation, U.S. Naval Research Laboratory, Washington, DC, March 29, 1984.
6. “LCAO- $X\alpha$ Calculation of Some Electronic Properties of Polyacetylene”, J. W. Mintmire, Quantum Chemistry Group, University of Uppsala, Sweden, December 8, 1982. (invited)
5. “Dielectric Properties of Polyacetylene”, J. W. Mintmire, Department of Chemistry, Odense University, Odense, Denmark, December 6, 1982. (invited)
4. “Electronic and Structural Properties of Polyacetylene”, J. W. Mintmire, Chemistry Division, U.S. Naval Research Laboratory, Washington, DC, October 5, 1982.
3. “Calculation of Electric Properties of Quasi-One-Dimensional Polymers: Applications to Polyacetylene”, J. W. Mintmire, Department of Chemistry, Cornell University, September 7, 1982.
2. “Electronic Band Structure of all-trans Polyacetylene”, J. W. Mintmire, U.S. Naval Research Laboratory, Washington, DC, February 24, 1982.
1. “LCAO- $X\alpha$ Methods for Two-Dimensionally Periodic Thin Films”, J. W. Mintmire, Chemistry Division, U.S. Naval Research Laboratory, Washington, DC, April 3, 1980.

Service

National and International

- Co-Organizer, Nanomechanics Minisymposium, 3rd Canadian Conference on Nonlinear Solid Mechanics (CanCNSM2008), Toronto, ON, Canada, June 25-29, 2008.
- Participant, DAAD Information Tour 2007, December 2-8, 2007 visiting scientific research facilities in southern Germany, sponsored by the German Academic Exchange Service (DAAD).
- Technical Advisory Committee, 2007 Nanoelectronic Devices for Defense & Security (NANO-DDS) Conference, Crystal City, VA, June 18-21, 2007.
- Co-Chair, Program Committee, Applied Diamond Conference/Nanocarbon 2005, Argonne National Laboratory, Argonne, IL, May 15-19, 2005.
- Associate Member, IUPAC Commission II.3 (High-Temperature Materials and Solid State Chemistry), 2000-2001.
- Chair, FY99 NRL Chemistry Division Colloquium Committee.
- Organized March 1997 APS Division of Materials Physics Focused Session on Fullerenes, Carbon Nanotubes, and Related Materials, St. Louis, MO, with R. Ruoff and J. Schilling.
- Organized November 1994 MRS Symposium on Science and Technology of Fullerene Materials, Boston, MA, with P. Bernier, D. S. Bethune, L.Y. Chiang, T.W. Ebbesen and R.M. Metzger.

Oklahoma State University

- Chair, Mathematics Department Head Search Committee, 2011
- Member, OSU Strategic Plan Implementation and Monitoring Committee, 2011
- Returning Officer, Computer Science Department Head Reappointment, 2010
- Member, Executive Committee, Oklahoma EPSCoR Network for Nanostructured Materials (NanoNet), 2003-2008
- Member, Oklahoma State University Sigma Xi Membership Committee, 2004-2007.
- Chair, University High-Performance Computing Committee, 2004-2007
- Chair, Computer Science Department Head Search Committee, 2006-2007.
- Member, A&S/CEAT Nanoscience Faculty Search Committee, 2005-2006.
- Member, Arts & Sciences College Safety Committee, 2004-2005.
- Member, University Search Committee (Assistant Vice President for Research and Director of the Office of Intellectual Property Management), 2004
- Chair, Oklahoma State University Regents Distinguished Research Award Selection Committee, 2004
- Member, University Search Committee (Associate Vice President for Research and Graduate Dean), 2003-2004
- Member, University Search Committee (IT Telecommunications Director), 2003-2004

Service on Grant Agency Review Panels

Feb 2011	NSF panelist
Jan 2010	DOE Graduate Research Fellowship review panel
Oct 2008	NSF International Materials Institute (IMI) proposal review panel
May 2008	NSF NNIN renewal site review panel
May 2007	DOE Ames Lab Condensed Matter Physics and Materials Chemistry onsite review panel
Mar 2007	DOE Hydrogen Fuel Initiative fuel cell panel
Dec 2006	NSF IGERT full proposal review panel
Apr 2006	DOE SciDAC-2 review panel
Feb 2002	NSF Nanoscience Interdisciplinary Research Team Panel
Dec 2000	NSF Nanoscale Science and Engineering Center Preproposal Panel
Feb 2000	NSF Information Technology Research Preproposal Panel
Nov 1999	NSF MRSEC Preproposal Panel
Nov 1998	Review panel, AFOSR FY99 MURI on “Computational Prediction and Design of Materials Properties”
Jan 1997	NSF SEP Postdoctoral Program Panel
Feb 1996	NSF DASC Postdoctoral Research Associate Panel
Jun 1992	NSF CARM Supplement Panel