

JOHN W. MINTMIRE, Professor

Department of Physics

Oklahoma State University

145 Physical Sciences Bldg II

Stillwater, OK 74078

Voice: (405) 744-5796, Fax: (405) 744-6811, Email: john.mintmire@okstate.edu

Web page: <http://physicscourses.okstate.edu/mintmire/>

EDUCATION

Dec 1980 Ph. D., Physics, University of Florida, Gainesville, FL

Mar 1976 B.S., Physics, University of Florida, Gainesville, FL

PROFESSIONAL EXPERIENCE

2003-present Associate Dean of Research, College of Arts & Sciences,
Oklahoma State University, Stillwater, OK

2001-2003 Head, Department of Physics, Oklahoma State University, Stillwater, OK

2001-present Professor of Physics, Oklahoma State University, Stillwater, OK

1983-2001 Research Physicist, Chemistry Division, US Naval Research Laboratory,
Washington, DC

1998-1999 Program Director, Materials Theory, Division of Materials Research,
National Science Foundation, Arlington, VA

1989-1990 Visiting Associate Professor, Department of Physics, Ohio State
University, Columbus, OH

1981-1983 NRC Postdoctoral Research Fellow at NRL, Washington, DC

Professional Societies and Activities

American Physical Society (Fellow)

American Association of Physics Teachers

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

RESEARCH

Dr. Mintmire's research interests over the last decade have focused on computational simulations in materials chemistry and physics, with specific emphasis on large-scale atomistic simulations of the electronic and structural properties of low-dimensional materials. In 1992 he and his coworkers at the Naval Research Laboratory predicted the metallic nature of armchair carbon nanotubes years before any experimental measurements that stimulated subsequent experimental efforts to measure the electronic properties of these novel materials. He has authored or coauthored more than 100 publications.

REPRESENTATIVE PUBLICATIONS

1. "Stability and Electronic Structure of Phosphorus Nanotubes," I. Cabria and J. W. Mintmire, *Europhys. Lett.* **65**, 82 (2004).
2. "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).
3. "Metallic and Semiconducting Narrow Carbon Nanotubes," I. Cabria, J.W. Mintmire, and C.T. White, *Phys. Rev. B* **67**, R121406 (2003).
4. "Stability of Narrow Zigzag Carbon Nanotubes", I. Cabria, J. W. Mintmire, and C. T. White, *Int. J. Quantum Chem.* **91**, 51-56 (2003).
5. "Fundamental Properties of Single-Wall Carbon Nanotubes," C. T. White and J.W. Mintmire, *J. Phys. Chem. B*, in press (2005) [DOI [10.1021/jp047416+](https://doi.org/10.1021/jp047416+)]
6. "Molecular Dynamics Simulations of the Oxidation of Aluminum Nanoparticles", S. Alavi, J. W. Mintmire, and D. L. Thompson, *J. Phys. Chem. B*, in press (2005). [DOI [10.1021/jp046196x](https://doi.org/10.1021/jp046196x)]
7. "Are Fullerene Tubules Metallic?" J. W. Mintmire, B. I. Dunlap, and C. T. White, *Phys. Rev. Lett.* **68**, 631 (1992).
8. "Universal Density of States for Carbon Nanotubes," J. W. Mintmire and C. T. White, *Phys. Rev. Lett.* **81**, 2506 (1998).
9. "Density of States Reflects Diameter in Nanotubes," C. T. White and J. W. Mintmire, *Nature* **394**, 29 (1998).
10. "First-Principles Band Structures of Armchair Nanotubes," J. W. Mintmire and C. T. White, *Appl. Phys. A* **67**, 65 (1998).
11. "Helical and Rotational Symmetries of Nanoscale Graphitic Tubules", C.T. White, D.H. Robertson, and J.W. Mintmire, *Phys. Rev. B.* **47**, 5485-5488 (1992).
12. "First-Principles Electronic Properties of Model Silicon-Based Quantum Wires", J.W. Mintmire, *J. Vac. Sci. Tech. A* **11**, 1733-1735 (1993).
13. "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).
14. "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).
15. "Theoretical Treatment of the Dielectric Response of all-trans Polyacetylene", J.W. Mintmire and C.T. White, *Phys. Rev. B* **27**, 1447 (1983).
16. "Local-Density Functional Approach to all-trans Polyacetylene", J.W. Mintmire and C.T. White, *Phys. Rev. B* **28**, 3283 (1983).
17. "Heteroatom Effects in Heterocyclic Ring Chain Polymers", J.W. Mintmire, C.T. White, and M.L. Elert, *Synth. Metals* **16**, 235 (1986).
18. "Conformation and Electronic Structure of Heterocyclic Chain Polymers", J.W. Mintmire, C.T. White, and M.L. Elert, *Synth. Metals* **25**, 109 (1988).
19. "Conformational Effects in Organopolysilanes: A First-Principles Approach", J.W. Mintmire, *Phys. Rev. B.* **39**, 13350 (1989).
20. "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).