

Xiaoguang Zhang

Senior R&D Staff
Computer Science and Mathematics Division and
Center for Nanophase Materials Sciences
Oak Ridge National Laboratory
(865) 241-0200
xgz@ornl.gov



Education

Beijing University, Beijing, China	Physics	B.S., 1983
Northwestern University, Evanston, Illinois	Physics	Ph.D., 1989

Research Interests

Transport theory based on first-principles electronic structures and applied to nano- and molecular electronics and spintronics, electronic band structure theory, surface and interface problems, condensed matter phenomena, numerical algorithms, and parallel computation.

Professional Experience

1995–p	R&D Staff, Computer Science and Mathematics Division and Center for Nanophase Materials Sciences, ORNL
1993–1995	Postdoctoral Associate, Computer Science and Mathematics and Center for Nanophase Materials Sciences, ORNL
1991–1993	Postdoctoral Scholar, University of Kentucky-Lexington
1990–1991	Postdoctoral Fellow, Lawrence Berkeley Laboratory

Professional and Synergistic Activities

Referee, *Physical Review B*, *Physical Review Letters*, *Applied Physics Letters*, *Journal of Magnetism and Magnetic Materials*, and *Journal of Physics D: Applied Physics*

Honors and Awards

2000	Co-recipient, Computer World Smithsonian 2000 Laureate, for first teraflop scientific application.
1998	Co-recipient, Gordon Bell Prize, 1998, for best supercomputer application.
1996	Lockheed Martin Energy Research Corp. 1996 Awards Night, R&D Achievement Award.

Selected Peer-Reviewed Publications (Author of > 100 articles in refereed journals and books):

“Nonequilibrium Green’s Function Study of Pd₄-Cluster-Functionalized Carbon Nanotubes as Hydrogen Sensors,” C. Cao, A. F. Kemper, L. Agapito, J.-W. Zhang, Y. He, A. Rinzler, H.-P. Cheng, X.-G. Zhang, A. Reily, R. Sanvito, and S. Sanvito, *Phys. Rev. B* **79**, 075127 (2009).

“Numerical Study of the Noise Power of a Carbon Nanowire Network,” C. Zhou and X.-G. Zhang, *Phys. Rev. B* **78**, 174307 (2008).

“Nucleotide Capacitance Calculation for DNA Sequencing,” J.-Q. Lu and X.-G. Zhang, *Biophys. J.* **95**, L60 (2008).

“Standing Friedel Waves: A Quantum Probe of Electronic States in Nanoscale Devices,” J.-Q. Lu, X.-G. Zhang, and S. T. Pantelides, *Phys. Rev. Lett.* **99**, 226804 (2007).

“Generalized Bloch Theorem for Complex Periodic Potentials: A Powerful Application to Quantum Transport Calculations,” X.-G. Zhang, K. Varga, and S. T. Pantelides, *Phys. Rev. B* **76**, 035108 (2007).

Work Performed Under Earlier BES Funding

“First-Principles Transversal DNA Conductance Deconstructed,” X.-G. Zhang, P. S. Krstic, R. Zikic, J. C. Wells, and M. Fuentes-Cabrera, *Biophys. J.* **91**, L4 (2006).

“First-Principles Theory of Tunneling Currents in Metal-Oxide-Semiconductor Structures,” X.-G. Zhang, Z.-Y. Lu, and S. T. Pantelides, *Appl. Phys. Lett.*, **89**, 032112 (2006).

“First-Principles Theory of Quantum Well Resonance in Double Barrier Magnetic Tunnel Junctions,” Y. Wang, Z.-Y. Lu, X.-G. Zhang, and X. F. Han, *Phys. Rev. Lett.* **97**, 087210 (2006).

Collaborators Outside ORNL During Past Two Years: L.-Q. Chen, Penn State University; M. Greenblatt, Rutgers University; M. Juijben, University of Twent; J. Junquera, University of Cantabria, Spain; A. Kholkin, University Aveiro, Portugal; Morozovska, National Institute, National Academy of Science, Ukraine; A. E. W. Plummer, Louisiana State University; R. Ramesh, Univesrity of California, Berkeley; B. J. Rodriguez, University College Dublin; L. Royburd, University of Maryland; A. D. Stiff-Roberts, S. Trolier-McKinstry, Penn State University; Duke D.B. Williams, Lehigh University; J. Zhou, University of Wyoming

Graduate and Postdoctoral Advisors: Prof. E. W. Plummer, University of Pennsylvania

Thesis Advisor and Postgraduate-Scholar Sponsor:

Graduate Students: J. Shin (2003–2007), Physics, University of Tennessee-Knoxville with E. W. Plummer

Postdoctoral Scholars: Nina Balke, Humboldt, Germany; Senli Guo, ORNL; Alexander Tselev, ORNL; Maxim Nikiforov, ORNL; Katyayani Seal, ORNL; Brian Rodriguez, Humboldt, Germany; Stephen Jesse, ORNL; Jing Zhou, University of Wyoming

Total Graduate Students Advised: 1

Total Postdoctoral Scholars Advised: 8