

CURRICULUM VITAE

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Education and Training

Ph.D. University of Cincinnati 1989
B.S. University of Cincinnati 1983

Professional Employment

2013-present	Louisiana State University, Full professor, Cain Department of Chemical Engineering and the Center for Computation Technology
2010-2012	Associate Director, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory
2004-2010	Distinguished Senior Research Staff, Computational Chemical Sciences Group, ORNL
2001-2004	Senior Research Staff, Computational Chemical Sciences Group, ORNL
1998-2001	Group Leader, Computational Condensed Matter Physics Group, ORNL
1992-1998	Research Staff, Computer Science Group, ORNL

Other Positions Held, and Affiliations

Intel Supercomputer Systems Division Recognition Award, 1994
Oak Ridge National Laboratory Scientific Achievement Award 1994
Oak Ridge National Laboratory Division Director's Award 1993
Oak Ridge National Laboratory Scientific Achievement Award 1991
National Academy of Sciences NRC Post Doctoral Fellow, 1990
IEEE Gordon Bell Award, 1990
Cray Research Gigaflop Award, 1990

Invention Disclosures/Patents

Invention disclosure ID 1037: "Coulomb Buffer as a Method for Adjusting Band Offset and Alignment at Semiconductor/Insulator and Semiconductor/Semiconductor Interfaces."

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Anion: Photoelectron Spectroscopy and Theoretical Investigations," *Journal of Chemical Physics* **143**, 224301 (2015)

11. Bhaskaran-Nair, K., Karol Kowalski, K., Moreno, J., Jarrell, M. and Shelton, W.A., "Equation of motion coupled cluster methods for electron attachment and ionization potential in polyacenes," *Chemical Physics Letters* **641**, 146 (2015)
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13. Varga T., Droubay T.C., Bowden M.E., Stephens S.A., Manandhar S., Shuttanandan V., Colby R.J., Hu D.H., Shelton W.A., Chambers S.A., "Strain-dependence of the structure and ferroic properties of epitaxial Ni_{1-x}Ti_{1-y}O₃ thin films grown on sapphire substrates," *Thin Solid Films*, **578**, 113, 2015.
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15. Kowalski, K., Bhaskaran-Nair and Shelton, W.A., "Coupled Cluster Green's Function Employing Modified Spectral Resolution of Similarity Transformed Hamiltonians," *Journal of Chemical Physics*, **141**, 094102, 2014
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31. Xu, Y., Getman, R.B., Shelton, W.A., and Schneider, W.F., "A first-principles investigation of the effect of Pt cluster size on CO and NO oxidation intermediates and energetics," *Physical Chemistry Chemical Physics* **10**, 6009, 2008.
32. Ortiz J.E., Shelton W.A., Mantic V., Criado R., Gray L.J., and Paris F., "A Parallel Domain Decomposition BEM Algorithm for Three-Dimensional Exponential Mode Superposition," *J. of Appl. Mech.*, 75, 051108-1-051108-8, 2008.
33. Xu, Y., Shelton, W.A. and Schneider, W.F., "Theoretical Aspects of Oxide Particle Stability and Chemical Reactivity," *Synthesis, Properties, and Applications of Oxide Nanomaterials*, Eds. Rodríguez, J.A. and Fernández-García, M., Wiley, Hoboken, NJ (2007).
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Collaboration and Affiliation

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2010	Predictive System Simulation Capability for Evaluating Safety and Performance of Batteries	ORNL Laboratory Directed Research and Development (LDRD) Fund	\$450K/yr.	Co-PI
2009	A hybrid continuous/discontinuous Galerkin formulation	ORNL Laboratory Directed Research and Development (LDRD) Fund	\$ 250K/yr.	Co-PI
2008	Computer Design and Predictive Simulation of High-Capacity, Cyclable, and Versatile Nanoporous Supercapacitors for Energy Storage Applications	ORNL Laboratory Directed Research and Development (LDRD) Fund	\$300K/yr.	Co-PI
2008	IAAA Algorithms	DOE Office of Science ASCR	\$3M/yr.	Part.
2006	Nuclear Structure and Low Energy Reactions	DOE Office of Science Nuclear Physics	\$21.6M	Co-PI
2006	Advanced Methods for Electronic Structure	DOE Office of Science BES-Chemical Sciences	\$400K	Co-PI
2005	Chemicals and Forest Products Industries of the Future: From Natural Gas to Ethylene via Methane Homologation and Ethane Oxidative Dehydrogenation	DOE's Energy Efficiency and Renewable Energy, Industrial Technologies Program	\$400K/yr	Co-PI

2004	Catalyst by Design	DOE-BES-DMSE & DOE-ASCR	\$400K over 3 years	Co-PI
2004	Microscale modeling	DOE's EERE Industrial Technologies Program, Office of Freedom CAR and Vehicle Technologies	\$100K/yr.	PI
2004	Ceramics	DOE-BES-DMSE	\$90K/yr.	Part.
2004	Chemical Sciences	DOE-BES-Chem. Sciences	\$90K/yr.	Part.
2004	AMS Program	DOE-ASCR-MICS	\$90K/yr.	Co-PI
2003	DOE-EERE Heavy Vehicles Program	DOE-EERE-Office of Heavy Vehicles Technology		
1997-99	DOE HPCC Grand Challenge II	DOE	\$3M/yr.	Co-PI
1992-96	DOE HPCC Grand Challenge I	DOE	\$3M /yr.	Part.