

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

1990-1992 National Academy of Sciences/NRC Postdoctoral Fellow
1987-1988 Research Assistant/Physics Department, University of
Bristol, Bristol, UK

Honors and Awards

Blue Obelisk Award, 2012
IEEE Gordon Bell Award, 2001 (Honorable Mention)
IEEE Gordon Bell Award, 1998
Computerworld Smithsonian Award, 2000
Supercomputing '96 High Performance Computing Challenge Award, 1996
Supercomputing '95 High Performance Computing Challenge Award, 1995
Oak Ridge National Laboratory Scientific Achievement Award, 1995

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."

Recently Organized National Meetings Symposium

Organized Spring 2012 ACS meeting symposium on Li-air/metal-air Batteries
Y. Xu, W.A. Shelton and J. Nørskov

Publications

1. Rivero, P., Meunier, V. and Shelton, W.A.,"Electronic structure and magnetic transitions in $\text{LaMnO}_3/\text{SrTiO}_3$," Scientific Reports (in preparation)
2. Rivero, P., Meunier, V. and Shelton, W.A.," Effect of the adsorption of inorganic molecules in hydrogenated surfaces of diamond from Hybrid Density Functional Calculations," Surface Science (in preparation)
3. Bhaskaran-Nair K, Sumpter B.G., Kowalski K. and Shelton W.A.,"The Role of Electron Attachment and Ionization Potential on the Excited State Properties of P3HT," Journal of Physical Chemistry B (in preparation)
4. Kowalski, K., Bhaskaran-Nair, K. and Shelton, W.A.,"Coupled Cluster Green Function and Accurate Self-Energies: A 1st Principles Approach for Excited States and Electron Transport," Journal of Chemical Theory and Computation (in preparation)
5. Carillo, J-M Y. Siebers Z., Kumar R. Matheson, M.A., Ankner, J.F., Goswami, M., Bhaskaran-Nair, K., Shelton, W.A. Sumpter, B.G. and Kilbey, S.M.,"Petascale Computational and Neutron Reflectometry Studies of the Morphology and the Molecular Interface of Active Layers in Bulk Heterojunctions," ACS Nano (submitted)
6. Harrison, R.J., Beylkin, G., Bischoff, F.A., Calvin, J.A., Fann, G.I., Fosso-Tande, J., Diego, G., Hammond, J.R., Hartman-Baker, R., Hill, J.C., Jia, J., Kottmann, J.S., Ou, Y., Ratcliff, L.E., Reuter, M.G., Richie-Halford, A.C., Romero, N.A., Sekino, H., Shelton, W.A., Sundahl, B.E., Thorton, W.S., Valeev, E.F., Azquez-Mayagoitia, A.V., Vence, N. and Yokoi, Y.," MADNESS: A Multiresolution, Adaptive Numerical Environment for Scientific Simulation," SIAM Journal on Scientific Computing (accepted)
7. Bhaskaran-Nair K, Kowalski K. and Shelton W.A.,"Coupled Cluster Green function methods: Models involving Single and Double Excitations," Journal of Chemical Physics (accepted)
8. Rivero, P., Meunier, V. and Shelton, W.A.," Uniaxial pressure-induced half-metallic ferromagnetic phase transition in LaMnO_3 ," Physical Review B **93**, 094409 (2016)
9. Rivero, P., Meunier, V. and Shelton, W.A.," Electronic, structural, and magnetic properties of LaMnO_3 phase transition at high temperature," Physical Review B **93**, 024111 (2016)
10. Bhaskaran-Nair, K., Valiev, M., Deng, S.H.M., Shelton, W.A., Kowalski, K., and Wang, X.-B.,"Probing Microhydration Effects on the Electronic Structure of the GFP Chromophore

- 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)
 12. Mendez J.H., Ekuma C.C., Wu Y., Fulfer B., Prestigiacomo C., Jarrell M., Moreno J., Shelton W.A., Young D.P., Adams P.W., Karki A., Jin R., Chan J.Y., DiTusa J.F., "Exploring the magnetic, thermodynamic, and electronic structure properties of metamagnetic Fe₃Ga₄," *Physical Review B*, **91** (2015).
 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.
 14. Bullard, Z., Costa Girão, E., Owens, J.R., Shelton, W.A., Meunier, V., "Improved All-Carbon Spintronic Device Design," *Scientific Reports*, **5**, 7634, 2015.
 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
 16. Bhaskaran-Nair, K. Kowalski, K. Moreno, J., Jarrell M. and Shelton W.A., "Equation of Motion Coupled Cluster Methods for Electron Attachment and Ionization Potential for Fullerenes C₆₀ and C₇₀," *Journal of Chemical Physics*, **141**, 074304, 2014
 17. Allu, S., Velamur Asokan B., Shelton, W.A., Philip B., and Pannala, S., "A Generalized Multi-Dimensional Mathematic Model for Charging and Discharging Processes in Supercapacitors," *J. of Power Sources*, **256**, 369-382, 2014.
 18. B., Varga T., Droubay T.C., Bowden M.E., Colby R. J., Manandhar S., Shuttanandan V., Hu D.H., Kabius B.C., Apra E., Shelton W.A., Chambers S.A., "Coexistence of weak ferromagnetism and polar lattice distortion in epitaxial NiTiO₃ thin films of the LiNbO₃-type structure," *J. Vac. Sci. Technol., B*, **31**, 030603, 2013.
 19. Varga T., Droubay T.C., Bowden M.E., Nachimuthu P., Shuttanandan V., Bolin, T.B., Shelton W.A., Chambers S.A., "Epitaxial growth of NiTiO₃ with a distorted ilmenite structure," *Thin Solid Films*, **520**, 5534-5541, 2012.
 20. Dathar G.K.P., Shelton W.A., Xu Y., "Trend in the Catalytic Activity of Transition Metals for the Oxygen Reduction Reaction by Lithium," *J. of Phys. Chem. Lett.* **3**, 891-895, 2012.
 21. Xu Y. and Shelton W.A., "Oxygen reduction by Lithium on model Carbon and Oxidized Carbon Structures," *Journal of the Electrochemical Society*, **158**, A1177-A1184, 2011.
 22. Shelton W.A., Apra E., Sumpter B.G., Saraiva-Souza A., Souza Filho A.G. Del Nero J. and Meunier V., "Theory of zwitterionic molecular-based organic magnets," *Chemical Physics Letters*, **511**, 294-298, 2011.
 23. Archibald R.K., Shelton W.A. and Fann G.I., "Adaptive Discontinuous Galerkin Methods with Multiwavelet Basis," *Applied Numerical Mathematics*, **61**, 879-890, 2011.
 24. Jones K.M., Kalinin S.V., Kolmakov A., Luk'yanchuk I. A., Meunier V., Proksch R., Shelton W. A., Strelcov E., Tselev A., "Mesoscopic Metal-Insulator Transition at Ferroelastic Domain Walls in VO₂," *ACS Nano*, **4**, 4412-4419, 2010.
 25. Xu Y., Shelton W.A., "O₂ reduction by lithium on Au(111) and Pt(111)," *Journal of Chemical Physics*, **133**, 024703, 2010.
 26. Park K.T., Meunier V., Pan M., Shelton W.A., Yu N.-H., and Plummer E.W., "Nanoclusters of TiO₂ Wetted with Gold," *Surface Science*, **20**, 3131, 2009.
 27. Jiang D.-E., Chen X.-Q., Luo W., and Shelton W.A., "From trans-polyacetylene to zigzagged graphene nanoribbons," *Chemical Physics Letters*, **483**, 120, 2009.

28. Fann G.I., Pei J.C., Harrison R.J., Jia J., Hill J.C., Ou M.J., Nazarewicz W., Shelton W.A. and Schunck N., "Fast multiresolution methods for density functional theory in nuclear physics," *Journal of Physics: Conference Series*, **180**, 012080, 2009.
29. Apra E., Harrison R.J., Shelton W.A., Tipparaju V., and Vazquez-Mayagoitia A., "Computational Chemistry at the Petascale: Are We There Yet?," *Journal of Physics: Conference Series*, **180**, 012027, 2009.
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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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35. Fann G.I., Harrison R.J., Beylkin G., Jia J., Hartman-Baker R., Ou M.J., Shelton W.A. and Sugiki S., "MADNESS applied to density functional theory in chemistry and nuclear physics," *Journal of Physics: Conference Series*, **78** U163-U167, 2007.
36. Narula C.K., Moses M.J., Xu Y., Blom D.A., Allard L.F., Shelton W.A. and Schneider W.F. "Catalysis by Design - Theoretical and Experimental Studies of Model Catalysts," *Nanotechnology for Automotive Applications*, Document number 2007-01-1018, SAE International, Detroit MI (2007)
37. Xu, Y., Shelton, W. A., and Schneider, W. F., "Thermodynamic equilibrium compositions, structures, and reaction energies of Pt_xO_y (x=1-3) clusters predicted from first principles," *Journal of Physical Chemistry B* **110**, 16591, 2006.
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51. Canning, A., Ujfalussy, B., Schulthess, T., Zhang, X.-G., Shelton, W. A. , Nicholson, D. M. C., Stocks, G. M., Wang, Y. and Dirks, T., “Parallel Multi-teraflops Studies of the Magnetic Structure of FeMn Alloys,” *Proceedings of IPDPS03*, IEEE Computing Society, Los Alamitos, CA, 2003.
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Graduate and Post-doctoral Advisors

F.J. Pinski (University of Cincinnati), G. Malcolm Stocks (Oak Ridge National Laboratory), Warren Pickett (University of California, Davis)

Synergistic Activities

Editorial Board Computational Science & Discovery (IOP) (2008-present),

Organized Spring 2012 ACS meeting symposium on Li-air/metal-air Batteries

Y. Xu, W.A. Shelton and J. Nørskov

Proposal (DOE, NSF, ORNL, PNNL) reviewer; Journal Referee including *Physical Review Letters*, *Physical Review B*, *Journal of Applied Physics*, *Journal of Physics: Condensed Matter*, *Journal of Physical Chemistry (A,B & C)*, *Catalysis Today*, *Journal of Chemical Physics*, *Computer Physics Communication*, etc.

National Academy of Sciences NRC Post Doctoral Fellow, 1990

Collaboration and Affiliation

Jens Nørskov (Stanford), Yang Shao-Horn (MIT), D.D. Johnson (Ames), K.Kowalski (PNNL), K. Lopata (LSU), Y. Xu (LSU), J. Zhang (LSU), J. DiTusa (LSU), R. Jin (LSU), J. Spivey (LSU), S. Ghosh (IIT), W.F. Schneider (U. Notre Dame), K. Park (Baylor), V. Antropov (Ames), B. Harmon (Ames), M. Weinert (U. Wisc.-Mil), V. Meunier (RPI), B. Sumpter (ORNL), R.J. Harrison (SUNY), P. Kent (ORNL), J.Z. Larese (U. of Tennessee), E. Aprà (PNNL), G.M. Stocks (ORNL), D.M. Nicholson (ORNL), M. Buongiorno Nardelli (UNT), M.D. Barnes (U. Mass), J. Bernholc (NCSU), F. Pinski (U. Cincinnati), I. Gould (Imperial College), S. Kalinin (ORNL), E.W. Plummer (LSU), M.J. Hoffmann (U. Karlsruhe), P. Becher (ORNL), G. Painter (ORNL), B. Ujfalussy (Research Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences), R. McKee (ORNL), G. Ceder (MIT), N. Shibata (U. of Tokyo), A. Canning (NERSC/LBNL), W.H. Butler (U. of Alabama), J. Swihart (U. of Indiana) and Y. Wang (PSC).

Graduate Students and Post-Doctoral Students

Post doctoral Students: Y. Xu (LSU), M.L. Drummond (UNT), A.V. Smirnov (ISU/Ames), S. Dag (LBNL) and Kiran Bhaskran Nair (LSU), Zhenhua Ning (UIUC), Pablo Rivero (Universitat de Barcelona)

Graduate Students: J. Bourgeois (LSU), Y. Zhang (LSU), D.A. Biava (UIUC), Suffian Kahn (UIUC), Dan Finkenstadt (USNA), Eric Hines (FAU) and Raymond Igahara (UTK), Ahmed Ismail (MIT, DOE-CSGF), Matt Coddington (Oak Ridge High School)

Funding Portfolio (selected)

YEAR	TITLE	SOURCE	AWARD	PI
2015	Excited-state and Dynamical Materials Properties (eMaPs): An integrated design framework	DOE Office of Science BES-DMSE	\$2,874K/yr	Co-PI (pending)
2014	Mapping and Manipulating Materials Phase Transformation Pathways	DOE Office of Science BES-DMSE	\$700K/yr	Co-PI
2014	Building Neutron Scattering Infrastructure in Louisiana for Advanced Materials	DOE Office of Science BES-DMSE	\$1,868K/yr	Co-PI
2011	Environmental Molecular Sciences Laboratory Operations	DOE Office of Science BER	\$39,853K/yr	PI
2010	Disordered-Mediated Properties of Functional Materials	DOE Office of Science BES-DMSE	\$300K/yr.	Co-PI
2010	Achieving Rechargeable Li-Air Batteries through Metal Oxide Electrocatalysts	ORNL Laboratory Directed Research and Development (LDRD) Fund	\$500K/yr.	Co-PI

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
2005	The Development of Integral and Partial Differential Equation Techniques for Computational Science"	DOE-ASCR-MICS	\$400K/yr	PI
2005	Multiscale Modeling Nanochemistry Chemistry Endstation	ORNL Laboratory Directed Research and Development (LDRD) Fund	\$300K/yr. \$300K/yr. \$300K/yr.	Co-PI Co-PI Co-PI
2004	Molecular Transport	DOE-BES-DMSE & DOE-ASCR	\$1M/yr.	Part.

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.