Bobby G. Sumpter

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Nanomaterials Theory Institute, CNMS
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Publications

Education

Oklahoma State University	Ph.D. 1987 Physical Chemistry
Southwestern Oklahoma State University	B.S. 1983 Chemistry (ACS Certified)

Professional Experience

2014–Present Deputy Director, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory (ORNL)
2013–Present Joint Faculty Professor, Bredesen Center for Interdisciplinary Research and Graduate Education, University of Tennessee
2013–Present ORNL Corporate Fellow
2009–Present Group Leader, Computational Chemical and Materials Sciences and Director of the Nanomaterials Theory Institute, Oak Ridge National Laboratory, (ORNL), Oak Ridge, Tennessee
2009–Present Distinguished Research Staff, ORNL, Oak Ridge, Tennessee
2006–2009 Senior Research Staff, Center for Nanophase Materials Sciences, ORNL, Oak Ridge, Tennessee
2003–2009 Senior Research Staff, Computer Science & Mathematics Division, ORNL, Oak Ridge, Tennessee
1992–2002 Research staff scientist, ORNL, Oak Ridge, Tennessee
1988–1992 Research Associate, UT/ORNL, Oak Ridge, Tennessee
1987–1988 Postdoctoral Research, Cornell University

Professional Activities, Honors, Awards:

Fellow American Physical Society
Member APS, MRS, AAAS, ACS, ACerS, INNS
2015-Present Vice Chair ORNL Corporate Fellows Council
2014-Present Vice Chair Corporate Fellows Scientific Advisory Council for the Computing and Computational Sciences Directorate
2014-Present, Organization of ORNL Soft Matter Council
2014 CNMS Distinguished scientific paper
2013 UT-Battelle Corporate Fellow
2012 Significant Event Award (CeLEST);
2012 Most distinguished scientific paper award (CSMD)
2012 Division Director Award (CNMS)

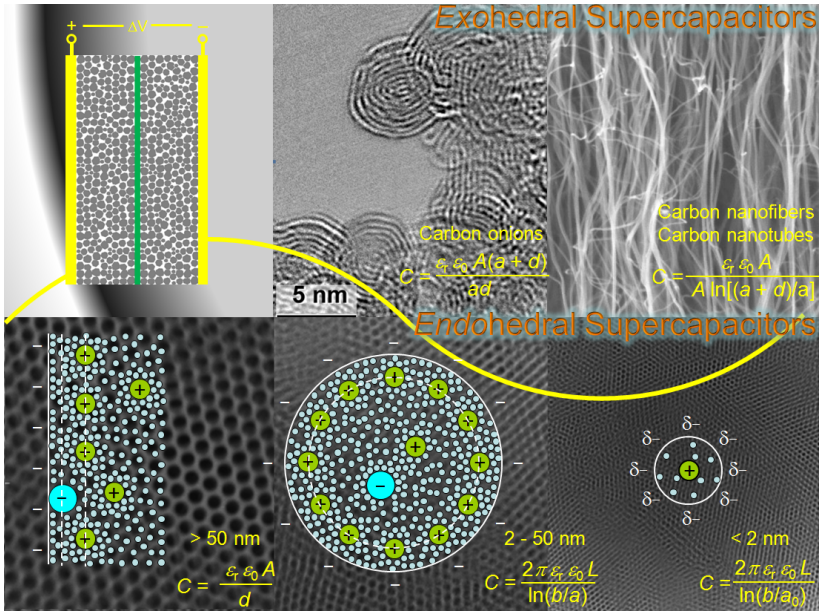
2009 Division Director Award (CNMS)
1999 Lockheed Martin Energy Research significant event award
1996 ORNL-CASD Technical Achievement award

Journal Editorial Board (prior)
Journal of Nanotechnology
International Journal of Smart Engineering System Design (previously)

Short Bio: Bobby G. Sumpter received his Bachelor of Science in Chemistry from Southwestern Oklahoma State University (1983) and a Ph.D. in Physical Chemistry from Oklahoma State University in 1987. Following postdoctoral studies in Chemical Physics at Cornell University 1987-1988 and in Polymer Chemistry at the University of Tennessee, Bobby joined the Chemistry Division at Oak Ridge National Laboratory in the Polymer Science group. He is currently the group leader for the Computational Chemical and Materials Sciences group and the Nanomaterials Theory Institute. Dr Sumpters' research is focused on the fundamental understanding of nanoscale self-assembly processes, interactions at interfaces, the structure and dynamics of molecular-based materials including multi-component polymers and composites, and the physical, mechanical and electronic properties of nanostructured materials.

Brief Research Synopsis

My research is directed primarily toward developing and applying modern computational and mathematical capabilities for the understanding and prediction of chemical and physical processes ranging from the molecular to the nanoscale to full-size engineering applications, using a multidisciplinary approach that integrates chemistry, physics, and materials science. Work is closely coupled with the experiments at the Center for Nanophase Materials Sciences (CNMS) and the Spallation Neutron Source (SNS), with a scientific focus on using theory and multiscale simulations and modeling for providing interpretive and predictive frameworks for virtual design and understanding of novel nanoscale materials with specific and/or emergent properties. The underlying goal is to ***understand, predict, design, control***, *and/or* ***exploit*** complex behavior that emerges at the nanoscale to enable capabilities that can lead to new innovations and improved materials for energy science and technology. Overall, this vision is aggressively pursued through a multi-pronged,



holistic, and tight integration with Oak Ridge National Laboratory distinctive capabilities in precision experimental synthesis and state-of-the-art characterization along side leadership class computing.

Research Areas/Topics:

(1) **Computational Soft Matter Science**: Unraveling the underlying multiscale physicochemical processes that control nanostructure morphologies and macroscopic physical, mechanical, electrical, and transport properties. Our goal is to understand how to design and control the nanoscale organization of macromolecular nanomaterials and their nanocomposites in order to achieve improved structure, properties, and functionality. Research highlights polymer-based materials for energy storage (supercapacitors and batteries), energy conversion (organic optoelectronics and photovoltaics), and lightweight structural materials (nanocomposites).

(2) **Surface/Substrate-Mediated Interactions, Interfaces, and Self-Assembly:** Understanding the mechanism(s) whereby unique assemblies of atoms and molecules are formed under realistic conditions to enable the design and synthesis of materials with prescribed functional (physiochemical) properties. We combine first-principles discovery and understanding enabled by high fidelity modeling/simulation with application of unique experimental methods for producing materials with nanometer scale structure (synthesis, surface patterning, layer deposition and nanostructuring, etc.) along with state-of-the-art tools for characterization, to study how intermolecular interactions and the complex correlations of atoms and molecules dictate the formation and properties of oriented nanostructures. This includes the effects of reduced dimensionality, confinement, and how substrates and support media or the environment interact with and induce changes to materials.

(3) **Nanostructured and Layered Materials:** Understanding how atomic scale structure, confinement, and quantum mechanical effects impact electronic processes within these nanostructures and across interfaces. Very thin sheets of a material can exhibit greatly enhanced properties such as increased electrical conductivity as compared with the bulk and are well suited for applications in new electronic devices, super-strong-light weight composite materials and for energy generation and storage. For these materials, we can reliably discover/predict structure-function-transport relationships.

(4) Cyber-Enabled Design of High Capacity Energy Storage Materials: Theory, computational modeling and simulation, to investigate materials electrochemical processes at the length and time scale where the underlying "behavior" is controlled. The goal is to perform research that will not only lead to predictive simulations but that will advance the basic understanding of energy storage systems. For example, we want to be able to screen new electrolytes or additives for high-voltage batteries for chemical stability and to design improved formulations based on the insight obtained. At the same time, we need to be able to model stress buildup during phase transitions in battery electrodes during charge/discharge cycles and to co-design materials and nanostructures to

diminish degradation.

(5) **"Virtual" Materials Characterization & Prediction**: A computational-based capability using input from (in-situ) experimental tools like X-ray, neutron, HTEM, scanning probes, various spectroscopies, and a purely first principles approach, to enable rapid structural and dynamical characterization: A step towards multi-modal, multi-physics fusion and deep data analytics. The thesis for this work is that structure and properties of molecules, solids, and liquids are direct reflections of the underlying quantum motion of their electrons, theoretical and computational science when performed in concert with experiments offers great opportunity toward helping solve some of the grand challenges in energy science. Modern facilities provide a direct means to address this capability, in terms of mathematics, computer science (leadership computing), and experimental imaging and characterization facilities.

Peer Reviewed Journal Publications:

1-250

1. Balaka Barkakaty, Bradley S. Lokitz, Bobby Sumpter, David Uhrig, Katie L. Browning, Ivana Karpisova, Kevin W. Harman, Ilia Ivanov, Jamie M. Messman, S. Michael Kilbey II, Tailoring solid polymer thin films for selective and reversible CO_2 capture-release at room temperature, *Macromolecules,* DOI: 10.1021/acs.macromol.5b02483 (2016).
2. Ming-Wei Lin, Houlong L. Zhuang, Jiaqiang Yan, Thomas Zac Ward, Alexander A. Puretzky, Christopher M. Rouleau, Zeng Gai, Liangbo Liang, Vincent Meunier, Bobby Sumpter, David B. Geohegan, David Mandrus, Kai Xiao, A Two-Dimensional $CrSiTe_3$ Ferromagnetic Material, *J. Mat. Chem. C.* DOI:10.1039/c5tc03463a (2016).
3. Wang, Jun; Bonnesen, Peter; Rangel, Eduardo; Vallejo, E.; Sanchez-Castillo, Ariadna; Cleaves, Henderson; Baddorf, Arthur; Sumpter, Bobby; Pan, Minghu; Maksymovych, Petro; Fuentes-Cabrera, Miguel, Supramolecular polymerization of a prebiotic nucleoside provides insights into the creation of sequence-controlled polymers, *Nature Sci. Rep.* 6:18891 (2016). DOI: 10.1038/srep18891
4. Alexander A. Puretzky, Liangbo Liang, Xufan Li, Kai Xiao, Bobby G. Sumpter, Vincent Meunier, and David B. Geohegan, Twisted $MoSe_2$ bilayers with variable stacking and interlayer coupling revealed by low-frequency Raman spectroscopy, *ACS Nano* **10**, 2736–2744 (2016). DOI: 10.1021/acsnano.5b07807
5. Shengxi Huang, Liangbo Liang, Xi Ling, Alexander A. Puretzky, David B. Geohegan, Bobby G. Sumpter, Jing Kong, Vincent Meunier, Mildred S. Dresselhaus, Low-Frequency Interlayer Raman Modes to Probe Interface of Twisted Bilayer MoS_2, *Nano Lett.*, **16**, 1435−1444 (2016). doi: 10.1021/acs.nanolett.5b05015
6. Nabankur Deb, Bohao Li, Maximilian Skoda, Sarah Rogers, Yan Sun, Xiong Gong, Alamgir Karim, Bobby G. Sumpter and David G Bucknall, Harnessing

Structure-Property Relationships for Poly(alkyl thiophene)-Fullerene Derivative Thin Films to Optimize Performance in Photovoltaic Devices, *Adv. Func. Mat.* (2016). DOI: 10.1002/adfm.201502653

7. Yadong He, Rui Qiao, Jenel Vatamanu, Oleg Borodin, Dmitry Bedrov, Jingsong Huang, Bobby G. Sumpter, The Importance of Ion Packing on the Dynamics of Ionic Liquids during nanopore charging, *J. Phys. Chem. Lett.,* **7**, 36−42 (2015). DOI: 10.1021/acs.jpclett.5b02378
8. Rajeev Kumar,Vera Bocharova, Evgheni Strelcov, Alexander Tselev, Ivan I. Kravchenko, Stefan Berdzinski, Veronika Strehmel, Olga S. Ovchinnikova, Joseph A. Minutolo, Joshua R. Sangoro, Alexander L. Agapov, Alexei P. Sokolov, Sergei V. Kalinin, Bobby G. Sumpter, Ion transport and softening in a polymerized ionic liquid, *Nanoscale* **7**, 947-955 (2015). DOI: 10.1039/c4nr05491a
9. Jewook Park, Jaekwang Lee, Lei Liu, Corentin Durand, Changwon Park, Mina Yoon, Bobby G. Sumpter, Arthur P. Baddorf, Gong Gu, and An-Ping Li, Spatially Resolved One-Dimensional Boundary States in Graphene-Hexagonal Boron Nitride Planar Heterostructures, *Nature Commun.* **5**:5403 (2015). DOI:10.1038/ncomms6403
10. Liangbo Liang, Jun Wang, Wenzhi Lin, Bobby G. Sumpter, Vincent Meunier, Minghu Pan, Electronic Bandgap and Edge Reconstruction in Phosphorene Materials, *Nano. Lett.* **16,** 6400-6406 (2015). DOI: 10.1021/nl502892t
11. Evgheni Strelcov, Rajeev Kumar, Vera Bocharova, Bobby G. Sumpter, Alexander Tselev, Sergei V. Kalinin, Nanoscale Lubrication of Ionic Surfaces Controlled via a Strong Electric Field, *Nature Sci. Reports*. **5**:8049 (2015). DOI: 10.1038/srep08049
12. Rajeev Kumar, Bradley S. Lokitz, Scott W. Sides, Jihua Chen, William T. Heller, John F. Ankner, Jim Browning, S. Michael Kilbey II, Bobby G. Sumpter, Microphase separation in thin films of lamellar forming polydisperse di-block copolymers, *RSC Advances* **5**, 21336 (2015). DOI: 10.1039/C5RA00974J
13. Che-Nan Sun, Thomas A. Zawodzinski Jr., Wyatt E. Tenhaeff, Fei Ren, Jong Kahk Keum, Sheng Bi, Dawen Li, Suk-Kyun Ahn, Kunlun Hong, Adam J. Rondinone, Karren L. More, Bobby G. Sumpter, Jihua Chen, Nanostructure Enhanced Ionic Transport in Fullerene Based Nanocomposite Electrolytes, *Phys. Chem. Chem. Phys.* **17**, 8266-8275 (2015). **DOI:** 10.1039/C4CP05583G
14. Evgheni Strelcov, Alexei Belianinov, Bobby G. Sumpter, Sergei V. Kalinin, Extracting Physics by Data Mining, *Materials Today* **17**, 416-417 (2015). DOI: 10.1016/ 416 j.mattod.2014.10.002
15. Jia Zhou, Bobby G. Sumpter, Paul R. C. Kent, Jingsong Huang, A Novel and Functional Single-Layer Sheet of ZnSe, *ACS Applied Materials & Interfaces 7***,** 1458–1464 (2015). 10.1021/am505655m
16. Ying Liu, Scott T. Huxtable, Bao Yang, Bobby G. Sumpter, Rui Qiao, Nonlocal Thermal Transport across Embedded Few-Layer Graphene Sheets, *J. Phys: Cond. Matter Fast Track* **26**, 502101 (2014). DOI: 10.1088/0953-8984/26/50/502101

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18. Yadong He, Peng Wu, Jingsong Huang, Bobby G. Sumpter, Alexei A. Kornyshev, Rui Qiao, Dynamic Charge Storage in Ionic Liquids-Filled Nanopores: Insight from a Computational Cyclic Voltammetry Study, *J. Phys. Chem. Lett.* **6**, 22−30 (2015). DOI: 10.1021/jz5024306
19. Changwon Park, Junga Ryou, Suklyun Hong, Bobby Sumpter, Gunn Kim, and Mina Yoon, Electronic properties of bilayer graphenes strongly coupled to interlayer stacking and an external field**,** *Phys. Rev. Lett.* **115**, 015502 (2015).
20. Jiahua Zhu, Youngkyu Han, Rajeev Kumar, Youjun He, Kunlun Hong, Peter Bonnesen, Bobby G. Sumpter, Changwoo Do, Sean Smith, Ilia Ivanov, Changwoo Do, Controlling Molecular-Ordering in Solution-State Conjugated Polymers, *Nanoscale* **7**, 15134-15141 (2015). **DOI:** 10.1039/C5NR02037A
21. Yong-Hui Tian, Jingsong Huang, Bobby G. Sumpter, Boron- and Nitrogen-Doped Phenalenyls: Unexpected 2e/ and 4e/all-sites pi-pi Covalency and Genuine Pancake Double Bonding, submitted. *J. Phys. Chem. Lett.* **6**, 2318−2325 (2015). DOI: 10.1021/acs.jpclett.5b00857
22. Nuradhika Herath, Sanjib Das, Jong K. Keum, Jiahua Zhu, Rajeev Kumar, Ilia N. Ivanov, Bobby G. Sumpter, James F. Browning, Kai Xiao, Gong Gu, Pooran Joshi, Sean Smith, Valeria Lauter, Peculiarity of Two Thermodynamically-Stable Morphologies and Their impact on the Efficiency of Solution-Processed Small Molecule Bulk Heterojunction Photovoltaic Devices, *Nature Sci. Reports,* **5:** 13407 (2015). DOI: 10.1038/srep13407
23. Yun Wang, Jingsong Huang, Bobby G. Sumpter, Haimin Zhang, Porun Liu, Huagui Yang, Huijun Zhao, Density Functional Studies of Stoichiometric Surfaces of Orthorhombic Hybrid Perovskite $CH_3NH_3PbI_3$, *J. Phys. Chem. C*., **119**, 1136-1145 (2015). DOI: 10.1021/jp511123s
24. Bing Huang, Houlong Zhuang, Mina Yoon, Su-Huai Wei, and Bobby G. Sumpter, Unexpected Stable Two-dimensional Silicon Phosphides with Different Stoichiometries, *Phys. Rev. B Rapid Commun.* **91**, 121401 (2015). DOI: 10.1103/PhysRevB.91.121401
25. Monojoy Goswami, Jose M. Borreguero, Bobby G. Sumpter, Self-assembly and structural relaxation in a model ionomer melt, *J. Chem. Phys.* **142**, 084903 (2015). DOI: 10.1063/1.4913517
26. Abdelaziz Boulesbaa, Bing Huang, Kai Wang, Ming-wei Lin, Masoud Mahjouri-Samani, Christopher Rouleau, Kai Xiao, Mina Yoon, Bobby Sumpter, Alexander Puretzky, David Geohegan, Observation of Two Distinct Negative Trions in Tungsten Disulfide Monolyayers, *PRB Rapid Commun*. **92**, 11543 (2015).
27. Yang Bai, Hui-Min He, Ying Li, Zhi-Ru Li, Zhong-Jun Zhou, Jia-Jun Wang, Di Wu, Wei Chen, Feng-Long Gu, Bobby G. Sumpter, Jingsong Huang, Electric Field Effects on the Intermolecular Interactions in Water Whiskers:

Insights from Structures, Energetics, and Properties, *J. Phys. Chem. A.* **119**, 2083-2090 (2015). DOI: 10.1021/jp511460c
28. S. Jesse, Q. He, A.R. Lupini, D.N. Leonard, M.P. Oxley, O. Ovchinnikov, R. Unocic, A. Tselev, M. Fuentes-Cabrera, B. G. Sumpter, S.J. Pennycook, S. V. Kalinin, A.Y. Borisevich, Atomic-level sculpting of crystalline oxides: towards bulk nanofabrication with single atomic plane precision, *Small* 11, 5895-5800 (2015). DOI: 10.1002/smll.201502048
29. Liangbo Liang, Xufan Li, Kai Xiao, Kai Wang, Masoud Mahjouri-Samani, Leonardo Basile, Juan Idrobo, Bobby G. Sumpter, Vincent Meunier, David B. Geohegan, Low-frequency Raman spectroscopy reveals stacking patterns of two-dimensional transition metal dichalcogenides, *ACS Nano* **9**, 6333–6342 (2015). DOI: 10.1021/acsnano.5b01884
30. Alexander A. Puretzky, Liangbo Liang, Xufan Li, Kai Xiao, Kai Wang, Masoud Mahjouri-Samani, Leonardo Basile, Juan Idrobo, Bobby G. Sumpter, Vincent Meunier, David B. Geohegan, Low-frequency Raman spectroscopy reveals stacking patterns of two-dimensional transition metal dichalcogenides, *ACS Nano* **9**, 6333–6342 (2015). DOI: 10.1021/acsnano.5b01884
31. Xi Ling, Liangbo Liang, Shengxi Huang, Alexander A. Puretzky, David B. Geohegan, Bobby G. Sumpter, Jing Kong, Vincent Meunier, Mildred S. Dresselhaus, Low-frequency Interlayer Breathing Modes in Few-layer Black Phosphorus, *Nano Lett.* **15**, 4080−4088 (2015). DOI: 10.1021/acs.nanolett.5b01117
32. Jan-Michael Y. Carrillo, Shiwang Cheng, Rajeev Kumar, Monojoy Goswami, Alexei P. Sokolov, Bobby G. Sumpter, Untangling the Effects of Chain Rigidity on the Structure and Dynamics of Strongly Adsorbed Polymer Melts, *Macromolecules* **48**, 4207−4219 (2015). DOI: 10.1021/acs.macromol.5b00624
33. Xufan Li, Leonardo Basile, Bing Huang, Cheng Ma, Jaekwang Lee, Ivan V. Vlassiouk, Alexander A. Puretzky, Ming-Wei Lin, Mina Yoon, Miaofang Chi, Juan C. Idrobo, Christopher M. Rouleau, Bobby G. Sumpter, David B. Geohegan, Kai Xiao, Van der Waals Epitaxy Growth of Large-Area, Two-Dimensional GaSe on Graphene, *ACS Nano* **9**, 8078-8088 (2015). DOI: 10.1021/acsnano.5b01943
34. Ying Liu, Chongze Hu, Jingsong Huang, Bobby G. Sumpter, Rui Qiao, Tuning Interfacial Thermal Conductance of Graphene Embedded in Soft Materials by Vacancy Defects, *J. Chem. Phys.* **142**, 244703 (2015) DOI: 10.1063/1.4922775
35. Yong-Hui Tian, Jingsong Huang, Bobby G. Sumpter, Miklos Kertesz, Nitrogen-Doping Enables Covalent-Like π−π Bonding between Graphenes, *Nano Lett.* **15**, 5482-5491 (2015). DOI: 10.1021/acs.nanolett.5b01940
36. Bing Huang, Mina Yoon, Bobby G Sumpter, Su-Huai Wei, Feng Liu, Alloy Engineering of Defect Properties in Semiconductors: Suppression of Deep Levels in 2D Transition-metal Dichalcogenides, *Phys. Rev. Lett.* **115**, 126806 (2015).
37. Colin Daniels, Andrew Horning, Anthony Phillips**,** Daniel V. P. Massote, Liangbo Liang, Zachary Bullard**,** Bobby G. Sumpter, Vincent Meunier**,** Mechanisms of Stress Release in Graphene Materials, *J. Phys: Cond. Matter*, **27**, 373002-373002 (2015).

38. S. Kalinin, B. G. Sumpter, R. Archibald, Big-Deep-Smart Data in Imaging for Guiding Materials Design, *Nature Materia*ls, **14**, 973-980 (2015). DOI: 10.1038/NMAT4395
39. Unocic, A. Tselev, M. Fuentes-Cabrera, B. G. Sumpter, S.J. Pennycook, S. V. Kalinin, A.Y. Borisevich, Atomic-level sculpting of crystalline oxides: towards bulk nanofabrication with single atomic plane precision, *Small* 11, 5895-5800 (2015). DOI: 10.1002/smll.201502048
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41. J. P. Mahalik, Y. Yang, Chaitra Deodhar, John F. Anker, Bradley S. Lokitz, S. Michael Kilbey, Bobby G. Sumpter, R. Kumar, Modeling a pH responsive weak polyelectrolyte planar brush using analytical and self-consistent field theory, *J. Poly. Sci. B.* accepted (2015).
42. Ganesh R Bhimanapati, Zhong Lin, Vincent Meunier, Judy Cha, Saptarshi Das, Di Xiao, Michael Strano, Valentino Cooper, Liangbo Liang, Steven G. Louie, Emilie Ringe, Wu Zhou, Bobby G. Sumpter Humberto Terrones, Fengnian Xia, Jun Zhu, Deji Akinwande, Nasim Alem, John Schuller, Raymond Schaak, Mauricio Terrones, Joshua A. Robinson, Recent Advances in 2D Materials Beyond Graphene, *ACS Nano*, **DOI:** 10.1021/acsnano.5b05556 (2015).
43. Seokmin Jeon, Peter Doak, Bobby G. Sumpter, Panchapakesan Ganesh, Petro Maksymovych, Electrostatic control of two-dimensional ionic molecular structures on metal surfaces, *ACS Nano*. accepted (2015).
44. Uma Tumuluri, Meijun Li, Brandon Cook, Bobby Sumpter, Sheng Dai, Zili Wu, Surface structure dependence of SO_2 interaction with ceria nanocrystals with well-defined facets, *J. Phys. Chem. C.* **119**, 28895–28905 (2015). DOI: 10.1021/acs.jpcc.5b07946
45. Jian Gao, Young-Duck Kim, Liangbo Liang, Juan-Carlos Idrobo, Phil Chow, Baichang Li, Jiawei Tan, Lu Li, Bobby G. Sumpter, Toh-Ming Lu, Vincent Meunier, James Hone, Nikhil Koratkar, Transition metal doping in synthetic atomically-thin semiconductors, *Nature Commun.* Under revision (2015).
46. Shiwang Cheng, Stephen Mirigian, Jan-Michael Y. Carrillo, Vera Bocharova,[1] Bobby G. Sumpter, Kenneth S. Schweizer, Alexei P. Sokolov, Revealing spatially heterogeneous relaxation in a model nanocomposite, *J. Chem. Phys.* 143, 194704 (2015); doi: 10.1063/1.4935595
47. Youngkyu Han, Jan-Michael Y. Carrillo, Zhe Zhang, Yunchao Li, Kunlun Hong, Bobby G. Sumpter, Mariappan Parans Paranthaman, Gregory S. Smith, Changwoo Do, Thermo-reversible morphology and conductivity of a conjugated polymer network embedded in polymeric self-assembly, Submitted (2015).
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Angle-Resolved Light-Matter Interaction in Anisotropic Layered Materials, *Nano Lett*., Submitted (2015).

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Acid-doped m-PBI Membranes, *J. Polym. Sci. B*. **52**, 26-35 (2014). DOI: 10.1002/polb.23403.

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61. Ming Shao, Jong Keum, Kunlun Hong, Jihua Chen, Youjun He, Wei Chen, James F. Browning, Jacek Jakowski, Bobby G. Sumpter, Ilia N. Ivanov, Ying-Zhong Ma, Christopher M. Rouleau, Sean C. Smith, David B. Geohegan, Kai Xiao, Untangling the isotopic effects of deuteration on the optoelectronic properties of conducting polymers, *Nature Commun*. **5**, 4180 (2014) DOI: 10.1038/ncomms4180
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Invited Books: Chapters and/or Editor

1. Jia Zhou, Humberto Terrones, Sean C. Smith, Bobby G. Sumpter, Jingsong Huang, Two-dimensional Layered Materials of ZnX and CdX (X = S, Se, Te), in "Beyond Graphene, New Layered Nanomaterials: Theory, Experiment and Applications", Wiley-VCH (2015).
2. Liangbo Liang, Bobby G. Sumpter, Vincent Meunier, Raman scattering of transition metal dichalcogenides, in "Beyond Graphene, New Layered Nanomaterials: Theory, Experiment and Applications", Wiley-VCH (2015).

3. R. Kumar, J. Carrillo, M. Goswami, B. G. Sumpter, “Insights obtained from modeling of organic photovoltaics: morphology, interfaces and coupling with charge transport,” in “Organic Solar Cells: Materials, Devices, Interfaces, and Modeling,” edited by Q. Qiao, CRC Press, Taylor and Francis Group (2015).
4. Bobby G. Sumpter, J.-M.Y. Carrillo, S.-K. Ahn, M. D. Barnes, W.A. Shelton, R.J. Harrison, D.W. Noid, “Development and Modeling of a Novel Self-Assembly Process for Polymer and Polymeric Composite Nanoparticles”, 2nd Edition of the book Nanotechnology in Biology and Medicine, published by CRC Press/Taylor & Francis Group, LLC (2015).
5. V. Meunier, E. Costa Girao, Bobby G. Sumpter “Modeling and simulation of electron transport at the nanoscale: Illustrations in low-dimensional carbon nanostructures”, pp 123-142, DOI:10.1007/978-3-642-33137-4_10 Springer-Verlag (2013).
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8. R. Kumar, J. Carrillo, M. Goswami, B. G. Sumpter, “Insights obtained from modeling of organic photovoltaics: morphology, interfaces and coupling with charge transport,” in “Organic Solar Cells: Materials, Devices, Interfaces, and Modeling,” edited by Q. Qiao, CRC Press, Taylor and Francis Group (2014).
9. Jingsong Huang, Ariana Beste, Jarod Younker, Alvaro Vazquez-Mayagoitia, Eduardo Cruz-Silva, Miguel Fuentes-Cabrera, Jacek Jakowski, Alejandro Lopez-Bezanilla, Vincent Meunier, Bobby G. Sumpter, “Advancing Understanding and Design of Functional Materials through Theoretical and Computational Chemical Physics”, in “Practical Aspects of Computational Chemistry II) Eds. J. Leszczynski and M.K. Shukla, Springer DOI 10.1007/978-94-007-0923-2_7 (2012).
10. E. C. Costa, B.G. Sumpter, V. Meunier, “Modeling and simulation of electron transport at the nanoscale: Illustrations in low-dimensional carbon nanostructures” Springer (2012).
11. E. C Gira, L. Liang, J. Owens, E. Cruz-Silva, B. G. Sumpter, V. Meunier, “Electronic Transport in Graphitic Carbon Nanoribbons”, Wiley (2012).
12. Alejandro Lopez-Bezanilla, Stephan Roche, Eduardo Cruz-Silva, Bobby G. Sumpter, and Vincent Meunier, “Electronic Transport in Carbon Nanomaterials”, Encyclopedia of Nanoscience and Nanotechnology, Springer (2012).
13. J. Huang, R. Qiao, Feng G, B.G. Sumpter, V. Meunier, “Modern theories of carbon-based electrochemical capacitors” in “Electrochemical capacitors: materials and systems”, Editor: François Béguin and Elzbieta Frackowiak, Wiley-VCH (2012).
14. Vincent Meunier, Bobby G. Sumpter, “Carbon Nanotube Memory Elements”, in Handbook of Nanophysics, CRC Press ISBN: 978-1-4200-7550-2 (2010).

15. Jingsong Huang, Bobby G. Sumpter, Vincent Meunier, “A Universal Model for Nanoporous Carbon Supercapacitors” in “Mesoporous Materials: Properties, Preparation and Applications”, ISBN**:** 978-1-60741-051-5 (2009).
16. M.L. Durmmond, B.G. Sumpter, M.D. Barnes, W.A. Sheltong, R.J. Harrision, “Using Nanoconfinement to Tailor Semiconducting Polymers: A combined Experimental and Multiscale Computational Study”, in “Multiscale Simulation Methods for Nanomaterials” Ed. By R.B. Ross and S. Mohanty (Wiley, 2008).
17. Bobby G. Sumpter, Vincent Meunier, “Optimizing the Electronic Properties of Carbon Nanotubes using Amphoteric Doping”**,** in “Multiscale Simulation Methods for Nanomaterials” Ed. By R.B. Ross and S. Mohanty (Wiley, 2008).
18. B.G. Sumpter, M.D. Barnes, W.A. Shelton, R.J. Harrison, D.W. Noid, “Development and Modeling of a Novel Self-Assembly Process for Polymer and Polymeric Nanoparticles”, in “Nanotechnology in Biology and Medicine: Methods, Devices, and Applications” Ed. By T. Vo-Dinh (CRC Press, 2007).
19. Bobby G. Sumpter, Donald W. Noid, Michael D. Barnes, Joshua U. Otaigbe, “Polymeric Nanoparticles”, in Encyclopedia of Nanoscience and Nanotechnology, American Scientific Publishers, ISBM: 9781588830012 (2004).
20. Bryan C. Hathorn, Donald W. Noid, Bobby G. Sumpter, Chao Yang, William A. Goddard III, “Computational Analysis Using Normal and Multibody Modes”**,** in Dekker Encyclopedia of Nanoscience and Nanotechnology, Second Edition, ISBN: 0-8493-9639-5 (2005).
21. “Computational studies, nanotechnology, and solution thermodynamics of polymer systems” edited by M.D. Dadmun, W. Alexander Van Hook, Donald W. Noid, Yuri B. Melnichenko and Bobby G. Sumpter, Kluwer Academic/Plenum Publishers, ISBM: 030646549 (2001).
22. “Molecular Simulation and Modeling of the Structure and Properties of Polymer Nanoparticles” in Computational studies, nanotechnology, and solution thermodynamics of polymer systems, Kluwer Academic/Plenum Publishers, ISBM: 030646549 (2001).
23. “Theory of the Production and Properties of Polymer Nanoparticles: Quantum Drops”, in Computational studies, nanotechnology, and solution thermodynamics of polymer systems, Kluwer Academic/Plenum Publishers, ISBM: 030646549 (2001).
24. “Shock and Pressure Wave Propagation in Nano-fluidic Systems”, in Computational studies, nanotechnology, and solution thermodynamics of polymer systems, Kluwer Academic/Plenum Publishers, ISBM: 030646549 (2001).
25. Bobby G. Sumpter, Robert E. Tuzun, and Donald W. Noid, "Computational simulation and modeling of polymeric materials", in *Multidimensional Molecular Dynamics Methods*, World Scientific Publishing Co., Inc. (1997).
26. Bobby G. Sumpter, Robert E. Tuzun, Donald W. Noid, “Computational Simulation and Modeling of Molecular-Based Materials”, in Modern Methods for Multidimensional Dynamics Computations in Chemistry, World Scientific, ISBN: 981-02-3324-6 (1998).
27. Robert E. Tuzun, Donald W. Noid, and Bobby G. Sumpter, "Recent advances in classical and quantum molecular simulation methods", in *Molecular dynamics of clusters, surfaces, liquids, and interfaces*, JAI Press (1999).

28. D.W. Noid, B.G. Sumpter, J.A. Darsey, B. Wunderlich and A. Xenopoulos, "Recent Advances in Molecular Dynamics Simulations: Applications to Polymer Crystals", in *Trends in Chemical Physics* published by the Council of Scientific Research Integration, 1, pp 207-238 (1991).
29. Coral Getino, Jesus Santamaria, Jerry A. Darsey and Bobby G. Sumpter, "Conformational Energy and Molecular Dynamics Studies of the Conducting Polymer Poly(Phenylenevinylene)", in *Computer Simulation of Polymers*, Chapter 2, pp 15-40 (1990).

Patents

US Patent 6,461,546, "*Apparatus for and method of producing monodisperse submicron polymer powders from solution,*" Oct. (2002).

Patents pending

US Patent Application 2009/0024,547 "*MULTI-INTELLIGENT SYSTEM FOR TOXICOGENOMIC APPLICATIONS (MISTA)"*

US Patent Application 12/758,930 "*Olefin-Containing Fuel Composition and Method*"

US Patent Application 13/860,291 "Self-assembly patterning of organic molecules on a surface"

Selected Recent Invited Talks

Bobby G. Sumpter, *Untangling complexity in functional polymeric materials through integrated simulation, synthesis and neutron scattering,* Materials Research Society Meeting, Boston, MA, Nov. 30-Dec.4, 2015.

Rajeev Kumar, Bobby G. Sumpter, *Theory-informed design of functional soft matter for energy science and technology*, ACS National Meeting & Exposition, Boston, MA, August 19, 2015.

Bobby G. Sumpter, *Polymers and Materials by Design*, Duke University, September 18 (2015).

Bobby G. Sumpter, *The Importance of Interfacial Dynamics in Polymer-Based Multicomponent Materials,* Stochastic Materials Workshop, Carey Institute for Global Good, Rensselaerville, NY (invited), Oct. 24-2 (2014).

Bobby G. Sumpter, *Interfacial Dynamics in Polymer-Based Multicomponent Materials,* Neutron Scattering in Soft Matter Workshop, Louisiana State University (invited), Dec. 8-9 (2014).

Bobby G. Sumpter, *Materials at Interfaces,* Frontiers in Data, Modeling and Simulation Workshop (invited), March 24-2 (2015), Argonne National Lab. [PTS: 55286]

"*The Importance of Interfacial Dynamics in Polymer-Based Multicomponent Materials",* Stochastic Materials Workshop, Carey Institute for Global Good, Rensselaerville, NW (invited), Oct. 24-2 (2014).

"*Interfacial Dynamics in Polymer-Based Multicomponent Materials",*Neutron Scattering in Soft Matter Workshop, Louisiana State University (invited), Dec. 8-9 (2014).

"*Nanostructured Materials: What's next and How Can Computational Science Help?"*, Materials Science and Physics Seminar, Rensselaer Polytechnic Institute, Oct. 9 Troy, NY (2014).

"*Computationally Guided Design of Nanostructured Soft Matter and Multicomponent Materials for Energy Science"*, Invited key note, Electronic Materials and Applications 2014 (American Ceramics Society), January 22-24, Orlando, FL (2014).

"*Understanding the origin of high-rate intercalation pseudocapacitance in* Nb_2O_5 *crystals"*, Electronic Materials and Applications 2014 (American Ceramics Society), January 22-24, Orlando, FL (2014)

"*Computationally Guided Design of Nanostructured Materials for Energy Science"*, Chemical and Biomolecular Engineering Department Seminar, University of Tennessee, March 4 (2014).

"*Functional Materials Discovery and Design for Energy Sciences"*, Invited Seminar, Southern Illinois University, Carbondale, IL April 17 (2014).

"*Large-Scale Simulations of Soft Matter and Multicomponent Materials for Energy Science Applications",* Grand Challenges in Soft Matter Workshop, University of California, Santa Barbara, May 18 (2014).

"*Nanostructured Soft Matter and Multicomponent Materials",* Gordon Research Conference, Mt. Snow, VT (invited **key note**), July 19 (2014).

"Computationally Guided Design of Nanostructured Soft Matter and Multicomponent Materials for Energy Science", Invited key note, Electronic Materials and Applications 2014 (American Ceramics Society), January 22-24, Orlando, FL (2014).

"Computationally Guided Design of Nanostructured Materials for Energy Science", Chemical and Biomolecular Engineering Department Seminar, University of Tennessee, March 4 (2014).

"Large-Scale Simulations of Soft Matter and Multicomponent Materials for Energy Science Applications", Grand Challenges in Soft Matter Workshop, UC Santa Barbara, May 17-18 (2014).

"Functional Materials Discovery and Design for Energy Sciences", Southern Illinois University, April 17 (2014).

"Nanomaterials Theory Institute and Computational Chemical and Materials Sciences", Duke University, March 12 (2013).

"Interfacial Compatibilizers and Buffer Layers for High Efficiency Organic Photovoltaics", Materials Research Society Meeting, November (2012).

"Computational Studies of Nanostructured Soft Matter and Multicomponent Materials for Energy Sciences", Center for Interdisciplinary Research and Graduate Education, October (2012).

"Nanostructured Soft Matter and Multicomponent Materials for Energy Sciences", Department of Physics and Astronomy Colloquium, University of Tennessee, September (2012)

"Nanostructured Soft-Matter Materials", Recent Advances in Materials Physics Symposium, NCSU, Raleigh, NC May (2012).

"Guiding the Design for Functional Materials for Energy S&T", Workshop on Opportunities for Accelerating Neutron Data Analysis, SNS, June (2012).

"Guiding the Design of Graphitic Materials for Efficient Energy Storage and Conversion", American Carbon Society Workshop, Stone Mountain, GA March 29-30 (2012).

"Exploring Structure-Property-Transport Relationships in Nanoscale Graphitic Systems", 2nd Annual EPSCoR Workshop, Knoxville,TN Oct. 10-12 (2011).

"Computational Insight for Guiding the Design of Nanostructured Materials", 20th Conference on Current Trends in Computational Chemistry, Jackson, MS, Oct. 27-29 (2011).

"Guiding the Design of Nanostructured Materials for Efficient Energy Storage, Conversion, and Transmission", Conference on Computational Physics 2011, Gatlingburg, TN, Oct. 30- Nov. 3 (2011).

"Design of Nanostructured Materials: Can Computational Science Help?", East Tennessee American Chemical Society meeting, Oak Ridge, TN, Nov. 8 (2011)

"Computational Exploration and Design of Functional Nanostructured Materials", Workshop on Modeling and Simulation of Materials in Soft Matter Science, Spallation Neutron Source Nov. 9-11 (2011).

"Simulation of Polymers in Complex Formulations", P&G workshop, Oak Ridge National Laboratory, Oct. 21 (2011).

"Modeling and Simulation of Interfacial Interactions and Processes", SOS15, Engelberg, Switzerland, March 14-16 (2011).

"Towards Understanding and Design of Functional Nanostructured Materials", Chemistry and Dynamics in Complex Environments Workshop, Telluride, Colorado, June 26-Juy 1 (2011).

"Self-assembly of charged-neutral diblock copolymers", American Chemical Society National Meeting, Denver Colorado, August 28- Sep. 2, (2011).

"Guiding the Design of Nanostructure Materials", HPC Forum, San Diego, California, Sep. 6-9 (2011).

"Nanoscale self-assembly and interfacial interactions", NSRC's Workshop: Theory and Simulation of Nano Scale Materials, Center for Integrated Nanotechnologies (CINT), Albuquerque, New Mexico, Oct. 14-15 (2010).

"Simulation and Modeling of the Structure and Dynamics of Multicomponent Polymeric Materials and Nanocomposites", Polymer Science and Engineering Department, University of Massachusetts Amherst, Dec. 9-10 (2010).

"Insights obtained from coarse-grained modeling of charged polymers", American Chemical Society SERMAC meeting, New Orleans, Dec. (2010)

"Design of advanced polymeric materials: can computer simulation help?", MARCO-2010, ITT Delhi, Dec. (2010).

"Towards Enabling the Guidance of Functional Materials Design", Workshop on Materials by Design, Oak Ridge National Laboratory, Sep. 20-21 (2011).

"Exploring Structure-Property Relationships of Nanaoscale Graphitic Systems", MRS International Meeting, Mexico August (2010)

"Self-Assembly and Nanoscale Confinement for Manipulating Structure and Properties of Materials", University of Tennessee, Chemistry/Materials/Physics seminar August (2010)

"Energy Storage and Conversion: How can Theory, Modeling, and Simulation Help", ORNL Symposium on Solar Energy and Energy Storage, September (2010)

"Theoretical and Computational Studies of Energy Conversion and Storage", University of Tennessee, Chemical and Biological Engineering Seminar, September (2010).

"Nanoscale Self-Assembly and Interfacial Interactions", NSRCs Theory Workshop, Albuquerque, New Mexico, (2010).
"Exploring Structure-Property Relationships in Nanoscale Graphitic Systems", MRS International meeting, Cancun Mexico, August 2010.

"Exploring Self-Assembly and the Fundamental Properties of Materials at Nanoscale Interfaces", colloquium at IPICyT, San Luis Potosi, Mexico (2009).

"Nanoscale Self-Assembly and the Fundamental Properties of Materials at Interfaces", Workshop on Organic Electronics and Spintronics, Nagoya Japan (2009).

"Using Self-assembly and Confinement for Manipulating Nanoscale Structure and Emergent Properties" CMOS Emerging Technologies Workshop, Canada (2010)

"Computational and Theoretical Nanoscience", Invited Lecture for CNMS educational outreach program, April (2010).

"Overview on the Next Generation Force Fields for Nanoscience", CNMS Workshop, Sep. (2010).

"On Exploring Structure-Function Relations at the Nanoscale: Energy Storage Applications", Ecuador, First International Nanotechnology Congress, Quito, Ecuador (2010)

"Theoretical and Computational Modeling of Carbon-Based Supercapacitors", 6th International Symposium on Computational Challenges and Tools for Nanotubes, Montreal, Canada (2010)

"Computational Modeling of Carbon Nanostructures for Energy Storage Applications", IEEE Nano 2010, Seoul, South Korea (2010)

"Theoretical and Computational Modeling of Carbon-Based Supercapacitors", ASME 2010 International Mechanical Engineering Congress, Vancouver, Canada, (2010)

"Theoretical and Computational Modeling of Carbon-Based Supercapacitors", Symposium on Research Opportunities in Electrochemical Energy Storage, Argonne, IL (2010)

"Theoretical and computational modeling of carbon-based supercapacitors", MRS Fall Meeting Boston (2009)

"Nanoscale self-assembly: manipulation and control of the structure, morphology and properties of materials", B. G. Sumpter, Workshop on Dynamics in Extreme Environments, Telluride, CO (2009).

"Manipulation and control of the structure, morphology and properties of heterostructures and carbon nanotubes", B. G. Sumpter, ACS National Meeting, Salt Lake City, UT (2009).

"Unconventional Donor-Acceptor Molecules for Supramolecular Assembly and Electronics", B. G. Sumpter, NSRC Contractors meeting, Annapolis, MA (2009).

"Capacitor Models for Various Regimes, Carbons and Electrolytes", Advanced Automotive Battery (AABC) conference, Long Beach, CA (2009)

"Dynamics and Structure of Multicomponent Polymeric and Nanocomposite materials", B. G. Sumpter, Proctor & Gamble (2009).

"Nanoscale Self-Assembly of Functional Materials", B. G. Sumpter, ACS Regional Meeting, Little Rock, AK (2008).

"Structure, Dynamics and Properties of Materials at the Nanoscale", B. G. Sumpter, IPICYT, Mexico (2008).

"Nanoscale Self-Assembly: Understanding and Control", B. G. Sumpter, ETSU, Department of Physics and Astronomy (2008).

"Nanoscale Self-Assembly of Functional Molecular Architectures", B. G. Sumpter, University of Mass., Amherst (2008).

"Towards Controlling the Growth of Carbon Nanotubes", B. G. Sumpter, Summer school on computational chemistry and materials science, Jackson MS (2008).

"Nanoscale self-assembly", B. G. Sumpter, Telluride Workshop on Complex Phenomena (2007).

"Computational Studies of Nanoscale Self-Assembly: A New Class of Supramolecular Wires", B. G. Sumpter, 15th Conference on Current Trends in Computational Chemistry, Jackson State University, Nov. (2006)

Recent Collaborations: Mike Barnes, Tom Russell– University of Massachusetts Amherst; Steven Stuart – Clemson University; Rui Qiao – Virginia Tech; Steven Gray– Argonne National Laboratory; Tuan Vo-Dinh, S. Curtarolo – Duke University; Jerry Darsey – University of Arkansas; William Goddard III – California Institute of Technology; Robert Tuzun – Suny Brockport; Chao Yang – Lawrence Berkeley National Laboratory; David Sherrill, J. L. Bredas, David Bucknell – Georgia Tech; Joshua Otaigbe – University of Southern Mississippi; Ronald Castellano – University of Florida; Scott Sides– National Renewable Energy Laboratory (NREL); Ed Valeev – Virginia Tech; J. Leszczynski – Jackson State University; David Keefer, Mark Dadmun, Jimmy Mays, Mike Kilbey – University of Tennessee; Martin Bakker – University of Alabama; Ian Gould – Imperial College London, M.S. Dresselhaus – MIT; M. Terrones – Penn State University; M. Endo – Shinshu University; A. Filho – Universidade Federal do Ceara;

F. Banhart, Universite de Strasbourg; J. Sponer – Academy of Sciences of Czech Republic; F.J. Luque – Universitat de Barcelona; Marco Nardelli – North Texas; Jerry Bernholc – NCSU; Vincent Meunier– Rensselaer Polytechnic Institute (RPI); Mauricio Terrnones – RPI; P.M. Ajayan – Rice University; A. Avgeropoulos–University of Ioannina, Greece

Graduate and Postdoc Advisors:
Graduate Advisor: Donald L. Thompson (U. Missouri- Columbia)
Postdoctoral Advisors: Greg S. Ezra (Cornell University), Bernhard Wunderlich (University of Tennessee, ORNL)

Postdoctoral Scholars Mentored (recent):
Michael Drummond (University of North Texas)
De-en Jiang (University of California, Riverside)
Jingsong Huang (Oak Ridge National Laboratory)
Alejandro Lopez-Benzanilla (Argonne National Lab)
Eduardo Cruz-Silva (Penn. State University)
Rajeev Kumar (Oak Ridge National Laboratory)
Jan-Michael Carrillo (Joint Institute for Computational Sciences, University of Tennessee & ORNL)
Jyoti Mahalik (Oak Ridge National Laboratory)

Graduate Student Mentorship: I have served on the committees and/or co-advised 5 Ph.D. students at the University of Tennessee (Department of Chemistry: Diaz Linton, William Carlen, Jacob Fasso-Tande), at Clemson University (Department of Chemistry: Pamala Piotrowsk), and the University of Arkansas (Department of Chemistry: William Griffin). Additionally, I have served on the committees and co-advised 2 International graduate students in the Advanced Materials Department at the Instituto Potosino de Investigación Científica y Tecnológica in San Luis Potosi, Mexico (Jessica Campos-Delgado and Eduardo Cruz-Silva). Currently I am mentoring, Artem Maksov (Ph.D. student at the University of Tennessee in the Bredesen Center for Interdiscplinary Graduate Education and Brandon P Plaisance (Ph.D. student at Georgia Institute of Technology and part of the ORNL Graduate Opportunities program)

Summer Student/Interns: Through ORAU/ORISE I consistently mentor a large number of summer students and visitors (on average 5 students each summer).