Bobby G. Sumpter

Deputy Director Center for Nanophase Materials Sciences (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

2017–present: Chair ORNL Corporate Fellows Council
2015-present: Interim Group Leader, Macromolecular Nanomaterials, Oak Ridge National Laboratory
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
Fellow of the American Association for the Advancement of Science
Member APS, MRS, AAAS, ACS, ACerS, INNS
UT-Battelle outstanding Mentor of Early Career Researchers award 2017
2015-2017 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

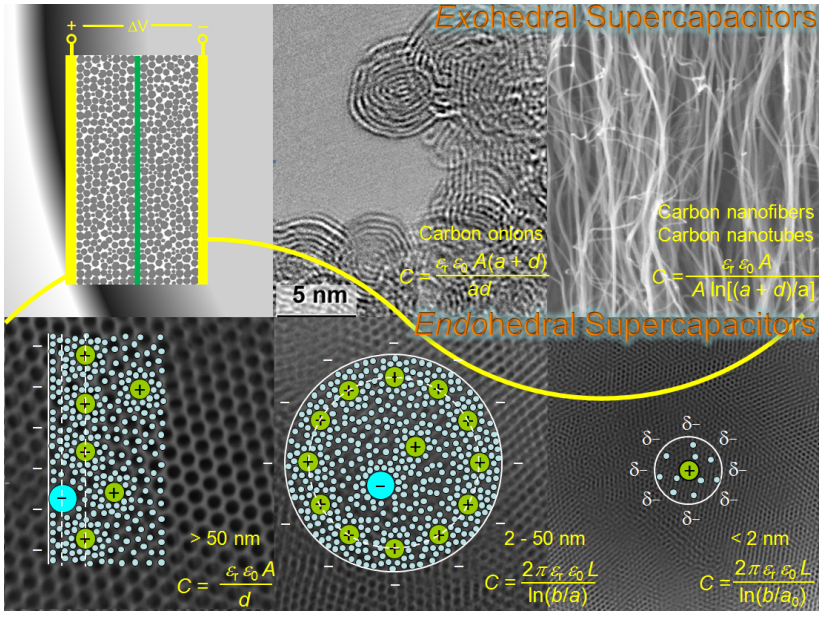
2014 CNMS Distinguished scientific paper
2013 UT-Battelle Corporate Fellow
2012 Significant Event Award (CeLEST);
2012 Most distinguished scientific paper award (CSMD)
2012 Division Director Award (CNMS)
2009 Division Director Award (CNMS)
1999 Lockheed Martin Energy Research significant event award
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 Sumpter's 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 alongside 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 and neutron scattering, (S)TEM, scanning probes, various spectroscopies, and a purely first principles approaches, 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, therefore theoretical and computational science when performed in concert with experiments can enable inroads toward solving 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 (h-index = 60 Google scholar):

1-250

1. Y. Song, D. Johnson, R. Peng, D. K. Hensley, P. V. Bonnesen, L. Liang, J. Huang, F. Yang, F. Zhang, R. Qiao, T. J. Tschaplinski, N. L. Engle, Z. Wu, D. A. Cullen, H. M. Meyer III, B. G. Sumpter, A. J. Rondinone, A Physical Catalyst for the Electrolysis of Nitrogen to Ammonia, *Science Adv*. (2018).
2. Yong-Hui Tian, Shuangli Hu, Xiaolan Sheng, Yixiang Duan, Jacek Jakowski, Bobby G. Sumpter, Jingsong Huang, Non-Transition Metal Catalytic System for N2 Reduction to NH3: A DFT Study of Al-Doped Graphene, *J. Phys. Chem. Lett.* **9,** 570-576 (2018).
3. Jyoti P. Mahalik, Jason Dugger, Scott W. Sides, Bobby G. Sumpter, Valeria Lauter, Rajeev Kumar, Modeling neutron reflectivity profiles of diblock copolymer nanocomposites using hybrid particle-field simulations, *Macromolecules* (2018). DOI: 10.1021/acs.macromol.8b00180
4. Chongze Hu, Peter Ni, Li Zhan, Huijuan Zhao, Jian He,Terry M. Tritt, Jingsong Huang, Bobby G. Sumpter, Theoretical Investigations of Electrical Transport Properties in $CoSb_3$ Skutterudites Under Hydrostatic Loadings, *Rare Metals* **37,** 316-325 (2018)
5. Sergey Chernyy, Jacob Judas Kain Kirkensgaard, Jyoti P. Mahalik, Hyeyoung Kim, Matthias ML Arras, Rajeev Kumar, Bobby G. Sumpter, Gregory S. Smith, Kell Mortensen, Thomas P. Russell, Kristoffer Almdal, Bulk and surface morphologies of ABC miktoarm star terpolymers comprised of PDMS, PI and PMMA arms, *Macromolecules* **51,** 1041-1051 (2018).
6. Wen-Sheng Xu, Jan-Michael Y. Carrillo, Christopher N. Lam, Bobby G. Sumpter, Yangyang Wang, Molecular Dynamics Investigation of the

Relaxation Mechanism of Entangled Polymers after a Large Step Deformation, *ACS Marco Lett*. **7,** 190-195 (2018).

7. Songkil Kim, Anton V. Ievlev, Jacek Jakowski, Xiahan Sang, Ivan V. Vlassiouk, Chance Brown, Ondrej Dyck, Raymond R. Unocic, Sergei V. Kalinin, Alex Belianinov, Bobby G. Sumpter, Stephen Jesse, Olga S. Ovchinnikova, Multi-Purposed Ar Gas Cluster Ion Beam Processing For Graphene Engineering, *Carbon* **131**, 142-148 (2018).
8. John Cummings, John S. Lowengrub, Bobby G. Sumpter, Steven M. Wise, Rajeev Kumar, Modeling solvent evaporation during thin film formation in phase separating polymer mixtures, *Soft Matter* **14**, 1833-1846 (2018).
9. Naisheng Jiang, Mani Sen, Wenduo Zeng, Zhizhao Chen, Maya K. Endoh, Tadanori Koga, Masafumi Fukuto, Guangcui Yuan, Sushil K. Satija, Jan-Michael Y. Carrillo, Bobby G. Sumpter, Structure-induced switching of interpolymer adhesion by polymer chains adsorbed onto a planar solid, *Soft Matter* **14**, 1108-1119 (2018).
10. Umi Yamamoto, Jan-Michael Y Carrillo, Vera Bocharova, Alexei P Sokolov, Bobby G Sumpter, Kenneth S Schweizer, Theory and Simulation of Attractive Nanoparticle Transport in Polymer Melts, *Macromolecules* (2018). **DOI:** 10.1021/acs.macromol.7b02694
11. Bobby Carroll, Vera Bocharova, Jan-Michael Y Carrillo, Alexander Kisliuk, Shiwang Cheng, Umi Yamamoto, Kenneth S Schweizer, Bobby G Sumpter, Alexei P Sokolov, Diffusion of Sticky Nanoparticles in a Polymer Melt: Crossover from Suppressed to Enhanced Transport, *Macromolecules* (2018). **DOI:** 10.1021/acs.macromol.7b02695
12. Liangbo Liang, Alexander A. Puretzky, Bobby G. Sumpter, Vincent Meunier, Interlayer bond polarizability model for stacking-dependent low-frequency Raman scattering in layered materials, *Nanoscale* **9**, 15340 - 15355 (2017).✔ DOI: 10.1039/C7NR05839J
13. Niranji Thilini Ekanayake, Jingsong Huang, Jacek Jakowski, Bobby G. Sumpter, Sophya Garashchuk, Relevance of the nuclear quantum effects on the proton/deuteron transmission through hexagonal boron nitride and graphene monolayers, *J. Phys. Chem. C.* **121**, 24335-24344 (2017). DOI: 10.1021/acs.jpcc.7b08152
14. Liangbo Liang, Jun Zhang, Bobby G. Sumpter, Qing-Hai Tan, Ping-Heng Tan,Vincent Meunier, Low-frequency Shear and Layer-Breathing Modes in Raman Scattering of Two-Dimensional Materials, *ACS Nano* **11**, 11777-11802 (2017). DOI: 10.1021/acsnano.7b06551
15. V. Bocharova, Z. Wojnarowska, P. Cao1, Y. Fu, R. Kumar, V. N. Novikov7, S. Zhao, A. Kisliuk, T. Saito, Jimmy W. Mays, B.G. Sumpter, A. P. Sokolov, The Influence of Chain Rigidity and Dielectric Constant on the Glass Transition Temperature in Polymerized Ionic Liquids, *J. Phys. Chem.* **121**, 11511-11519 (2017).
16. Chongze Hu, Jingsong Huang, Bobby G. Sumpter, Efstathios Meletis, Traian Dumitrică, *Ab Initio* Predictions of Hexagonal Zr(B,C,N) Polymorphs for Coherent Interface Design, *J. Phys. Chem. C.* **121,** 26007-26018 (2017). DOI: 10.1021/acs.jpcc.7b09444

17. Abdelaziz Boulesbaa, Kai Wang, Masoud Mahjouri-Samani, Mengkun Tian, Alexander A. Puretzky, Ilia Ivanov, Christopher M. Rouleau, Kai Xiao, Bobby G. Sumpter and David B. Geohegan, Ultrafast Formation of Weakly Bound Hybrid Excitons in 2D/0D Heterostructures, *J. Amer. Chem. Soc.* **138**, 14713–14719 (2017). **DOI:** 10.1021/jacs.6b08883
18. Akinola Oyedele, Shize Yang, Liangbo Liang, Alexander A. Puretzky, Kai Wang, Jingjie Zhang, Peng Yu, Pushpa R. Pudasaini, Avik W. Ghosh, Zheng Liu, Christopher M. Rouleau, Bobby G. Sumpter, Matthew F. Chisholm, Wu Zhou, Philip D. Rack, David B. Geohegan, Kai Xiao, PdSe2: Pentagonal Puckered 2D Layers with High Air Stability for Electronics, *J. Amer. Chem. Soc.* (2017). DOI: 10.1021/jacs.7b04865
19. Jaekwang Lee, Bobby G. Sumpter, Mina Yoon, Strain-engineered optoelectronic properties of two-dimensional transition metal dichalcogenide lateral heterostructures, *2D Materials* **4**, 021016 (2017). **DOI**: 10.1088/2053-1583/aa5542
20. Chuanxu Ma, Zhongcan Xiao, Honghai Zhang, Liangbo Liang, Jingsong Hunag, Wenchang Lu, Kunlun Hong, Bobby G. Sumpter, Jerry Bernholc, An-Ping Li, Controllable conversion of quasi-freestanding polymer chains to graphene nanoribbons, *Nature Comm.* **8**:14815, (2017). DOI: 10.1038/ncomms14815
21. Michael G. Stanford, Pushpa R. Pudasaini, Elisabeth T. Gallmeier, Nicholas Cross, Liangbo Liang, Akinola Oyedele, Gerd Duscher, Masoud Mahjouri-Samani, Kai Wang, Kai Xiao, David B. Geohegan, Alex Belianinov, Bobby G. Sumpter, Philip D. Rack, Transition-Metal Substitution Doping in Synthetic Atomically Thin Semiconductors *Adv. Func. Mater.* 1702829 (2017). DOI: 10.1002/adfm.201702829
22. Kuan Huang, Liangbo Liang, Songhai Chai, Uma Tumuluri, Meijun Li, Zili Wu, Bobby G. Sumpter, Sheng Dai, Aminopolymer Functionalization of Boron Nitride Nanosheets for Highly Efficient Capture of Carbon Dioxide, *Journal of Materials Chemistry A*, 5, 16241-16248 (2017) DOI: 10.1039/c7ta00644f
23. Shiwang Cheng, Shi-Jie Xie, Jan-Michael Carrillo, Bobby Carroll, Halie Martin, Mark Dadmun, Bobby G. Sumpter, Vladimir Novikov, Kenneth S. Schweizer, Alexei P. Sokolov, Big Effect of Small Nanoparticles: A New Paradigm for Polymer Nanocomposites, *ACS Nano*. **11**, 752–759 (2017). DOI: 10.1021/acsnano.6b07172
24. Shiwang Cheng, Bobby Carroll, Wei Lu, Fei Fan, Jan-Michael Carrillo, Halie Martin, Adam P. Holt, Nam-Goo Kang, Vera Bocharova, Jimmy W. Mays, Bobby G. Sumpter, Mark Dadmun, Alexei P. Sokolov, The role of chain rigidity in the interfacial properties of polymer nanocomposites, *Macromolecules*, **50**, 2397-2406 (2017). DOI: 10.1021/acs.macromol.6b02816
25. Suk-kyun Ahn, Jan-Michael Carrillo, Jong K. Keum, Jihua Chen, David Uhrig, Bradley S. Lokitz, Bobby G. Sumpter, S. Michael Kilbey II, Nanoporous Poly(3-hexylthiophene) Thin Film Structures from Self-Organization of a Tunable Molecular Bottlebrush Scaffold, *Nanoscale* **9**, 7071-7080 (2017). 10.1039/C7NR00015D

26. Eric S. Muckley, Christopher B. Jacobs, Keith Vidal, Jyoti P. Mahalik, Rajeev Kumar, Bobby G. Sumpter, Ilia N. Ivanov, New insights on electro-optical response of PEDOT:PSS film to humidity, *ACS Appl. Mater. & Interf*aces ***9***, 15880-15886 (2017). DOI: 10.1021/acsami.7b03128
27. Weili Cui, Shanshan Xu, Bo Yan, Zhihua Guo, Qun Xu, Bobby G. Sumpter, Jingsong Huang, Shiwei Yin, Huijun Zhao, and Yun Wang, Triphasic 2D Materials by Vertically Stacking Laterally Heterostructured 2H-/1T′-MoS2 on Graphene for Enhanced Photoresponse, *Adv. Electronic Mater.*, **3,** 17000224 (2017). DOI: 10.1002/aelm.201700024
28. Chongze Hu, Xiaoyu Zeng, Yufei Liu, Menghan Zhou, Huijuan Zhao, Terry M. Tritt, Jian He, Jacek Jakowski, Paul R. C. Kent, Jingsong Huang, Bobby G. Sumpter, Effects of partial La filling and Sb vacancy defects on CoSb3 skutterudites, *Phys. Rev. B*, **95**, 165204 (2017) DOI: 10.1103/ PhysRevB.00.005200
29. Jan-Michael Y. Carrillo, Matthew E. Potter, Miles A. Sakwa-Novak, Simon H. Pang, Christopher W. Jones, Bobby G. Sumpter, Linking Silica Support Morphology to the Dynamics of Aminopolymers in Composites, *Langmuir* **33**, 5412–5422 (2017). DOI: 10.1021/acs.langmuir.7b00283
30. Adam Holewinski, Miles A Sakwa-Novak, Jan-Michael Y Carrillo, Matthew E Potter, Nathan Ellebracht, Gernot Rother, Bobby G Sumpter, Christopher W Jones, Aminopolymer Mobility and Support Interactions in Silica-PEI Composites for CO2 Capture Applications: A Quasielastic Neutron Scattering Study, *J. Phys. Chem. B.* **121**, 6721-6731 (2017). DOI: 10.1021/ acs.jpcb.7b04106
31. Jose M. Borreguero, Philip A. Pincus, Bobby G. Sumpter, Monojoy Goswami, Dynamics of Charged Species in Ionic-Neutral Block Copolymer and Surfactant Complexes, *J. Phys. Chem. B.* **121**, 6958-6968 (2017) DOI: 10.1021/acs.jpcb.7b05047
32. Jose M. Borreguero, Philip A. Pincus, Bobby G. Sumpter, Monojoy Goswami, Unraveling the Agglomeration Mechanism in Charged Block Copolymer and Surfactant Complexes, *Macromolecules* **50**, 1193-1205 (2017). DOI: 10.1021/acs.macromol.6b02319
33. Adam Sims, Mathew Jeffers, Saikat Talapatra, Kanchan Mondal, Sewa Pokhrel, Liangbo Liang, Xianfeng Zhang, Ana L. Elias, Bobby G. Sumpter, Vincent Meunier, Mauricio Terrones, Hydro-deoxygenation of CO on functionalized carbon nanotubes for liquid fuels production, *Carbon* **121**, 274-284v(2017). DOI: 10.1016/j.carbon.2017.05.094
34. Anton V. Ievlev, Jacek Jakowski, Matthew J. Burch, Vighter Iberi, Holland Hysmith, David C. Joy, Bobby G. Sumpter, Alex Belianinov, Raymond R. Unocic, Olga S. Ovchinnikova, Building with ions: towards direct write of platinum nanostructures using in situ liquid cell helium ion Microscopy, *Nanoscale* **9**, 12949–12956 (2017). DOI: 10.1039/c7nr04417h
35. J. P. Mahalik, Bobby G. Sumpter, Rajeev Kumar, Attraction between opposing planar dipolar polymer brushes, *Macromolecules* (2017) DOI: 10.1021/acs.langmuir.7b01566

36. Jacek Jakowski, Jingsong Huang, Sophya Garashchuk,Yingdong Luo, Kunlun Hong, Jong Keum, Bobby G. Sumpter, Deuteration as a Means to Tune Crystallinity of Conducting Polymers, *J. Phys. Chem. Lett.* **8**, 4333-4340 (2017) DOI: 10.1021/acs.jpclett.7b01803
37. Yao Fu, Vera Bocharova, Mengze Ma, Alexei P. Sokolov, Bobby G. Sumpter, Rajeev Kumar, Effects of counterion size and backbone rigiditiy on dynamics of ionic polymer melts and glasses, *Phys. Chem. Chem. Phys.* (2017). DOI: 10.1039/C7CP04249C
38. Eric S. Muckley, Christopher B. Jacobs, Keith Vidal, Nickolay V. Lavrik, Bobby G. Sumpter, Ilia N. Ivanov, Multi-mode humidity sensing with water-soluble copper phthalocyanine for increased sensitivity and dynamic range, *Nature Sci. Rep.* **7**, 9921(2017). DOI:10.1038/s41598-017-10401-2
39. Eric J. Young, Rodney Burton, Jyoti P. Mahalik, Bobby G. Sumpter, Miguel Fuentes-Cabrera, Cheryl A. Kerfeld, Daniel C. Ducat, Engineering the Bacterial Microcompartment Domain for Molecular Scaffolding Applications, *Frontiers in Microbiology* **8,** 1441 (2017) DOI: 10.3389/fmicb.2017.01441
40. Fei Zhang, Yadong He, Jingsong Huang, Bobby G. Sumpter, Rui Qiao, Multicomponent Gas Storage in Organic Cage Molecules, *J. Phys. Chem. C* **121**, 12426-12433 (2017). DOI: 10.1021/acs.jpcc.7b01260
41. Balaka Barkakaty, Bobby G. Sumpter, Ilia N. Ivanov, Matthew E. Potter, Christopher W. Jones, Bradley S. Lokitz, Emerging Technologies for Lowering Atmospheric Carbon, *Env. Tech & Innov.,* **7**, 30-43 (2017).
42. Shiwang Cheng, Shi-Jie Xie, Jan-Michael Carrillo, Bobby Carroll, Halie Martin, Mark Dadmun, Bobby G. Sumpter, Vladimir Novikov, Kenneth S. Schweizer, Alexei P. Sokolov, Big Effect of Small Nanoparticles: A New Paradigm for Polymer Nanocomposites, *ACS Nano*. **11**, 752–759 (2017). DOI: 10.1021/acsnano.6b07172
43. Jan-Michael Y. Carrillo, John Katsaras, Bobby G. Sumpter, Rana Ashkar, A computational approach to model neutron scattering data from lipid bilayers, J. *Chem. Theory & Comp.* (2017). **DOI:** 10.1021/acs.jctc.6b00968
44. Fei Zhang, Yadong He, Jingsong Huang, Bobby G. Sumpter, Rui Qiao, Multi-Component Gas Storage in Organic Cage Molecules, *J. Phys. Chem.*, (2017). DOI: 10.1021/acs.jpcc.7b012
45. Rajeev Kumar, Jyoti Mahalik, Vera Bocharova, Eric Stacy, Catalin Gainaru, Tomonori Saito, Mallory Gobet, Steve Greenbaum, Bobby Sumpter, Alexei Sokolov, A Rayleighian approach for modeling kinetics of ionic transport in polymeric media, *J. Chem. Phys.* **146**, 064902 (2017).
46. Liangbo Liang, Alexander A. Puretzky, Bobby G. Sumpter, Vincent Meunier, Interlayer bond polarizability model for stacking-dependent low-frequency Raman scattering in layered materials, *Nanoscale* accepted (2017)
47. Konstantinos Misichronis, Jihua Chen, Adam Imel, Rajeev Kumar, James Thostenso, Kunlun Hong, Mark Dadmun, Bobby G. Sumpter, Justin G. Kennemur, Nikos Hadjichristidis, Jimmy W. Mays, Apostolos Avgeropoulos, Investigation on the Phase Diagram and Interaction Parameter of Poly(styrene-b-1,3-cyclohexadiene) Diblock Copolymers, *Macromolecules* **50**, 2354-2363 (2017).DOI: 10.1021/acs.macromol.7b00104

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49. Eric S. Muckley, Christopher B. Jacobs, Keith Vidal, Jyoti P. Mahalik, Rajeev Kumar, Bobby G. Sumpter, Ilia N. Ivanov, New insights on electro-optical response of PEDOT:PSS film to humidity, ACS Appl. Mater. & Interfaces ***9***, 15880–15886 (2017). DOI: 10.1021/acsami.7b03128
50. Weili Cui, Shanshan Xu, Bo Yan, Zhihua Guo, Qun Xu, Bobby G. Sumpter, Jingsong Huang, Shiwei Yin, Huijun Zhao, and Yun Wang, Triphasic 2D Materials by Vertically Stacking Laterally Heterostructured 2H-/1T′-MoS2 on Graphene for Enhanced Photoresponse, *Adv. Electronic Mater.*, 17000224 (2017). DOI: 10.1002/aelm.201700024
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55. V.E Lynch, J.M Borreguero, D. Bhowmik, B.G. Sumpter, T. Proffen, M. Goswami, An automated analysis workflow for optimization of force-field parameters using neutron scattering data, *J. Comp. Phys.* **340,** 128-137 (2017). DOI: 10.1016/j.jcp.2017.03.045
56. J. P. Mahalik, Bobby G. Sumpter, Rajeev Kumar, Vertical Phase Segregation Induced by Dipolar Interactions in Planar Polymer Brushes, *Macromolecules* **49**, 7096–7107 (2016). DOI: 10.1021/acs.macromol.6b01138
57. S. Jesse, Q. He, A. 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

58. 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
59. Emmanuel Vallejo, Miguel Fuentes-Cabrera, Bobby G. Sumpter, Eduardo Rangel Cortes, Isomeric effects on the self-assembly of a plausible prebiotic nucleoside analogue: A theoretical study, *Int. J. Quan. Chem.* **117**, 213–221 (2017). DOI: 10.1002/qua.25314
60. 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).
61. 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.* **4**, 315-322 (2016). DOI:10.1039/c5tc03463a
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Invited Books: Chapters and/or Editor

1. Valentino Cooper, Chris Lam, Yangyang Wang, B.G. Sumpter, Non-covalent interactions in nanotechnology, Elsevier (2017).

2. 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, CRC Press (2017).
3. 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 (2016).
4. 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 (2016).
5. 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).
6. 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).
7. 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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10. 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).
11. 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).
12. 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).
13. E. C Gira, L. Liang, J. Owens, E. Cruz-Silva, B. G. Sumpter, V. Meunier, "Electronic Transport in Graphitic Carbon Nanoribbons", Wiley (2012).

14. 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).
15. 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).
16. Vincent Meunier, Bobby G. Sumpter, "Carbon Nanotube Memory Elements", in Handbook of Nanophysics, CRC Press ISBN: 978-1-4200-7550-2 (2010).
17. 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).
18. 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).
19. 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).
20. 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).
21. 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).
22. 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).
23. "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).
24. "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).
25. "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).
26. "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).

27. 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).
28. 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).
29. 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).
30. 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).
31. 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).

US Patent 9,610,608 "*Self-Assembly Patterning of Organic Molecules on a Surface*", April 4, 2017.

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*"

Selected Recent Invited Talks

Bobby G. Sumpter, "*Porous organic cages as solvents with permanent porosity*", GaTech, March 23, 2017.

Bobby G. Sumpter, "*Polymers and Materials by Design"*, Georgetown University, July 2017.

Bobby G. Sumpter and Ilia Ivanov, "*Untangling and controlling complexity to enable tuned assembly in polymeric materials"*, MRS Cancun Mexico, August 2017.

Bobby G. Sumpter, "*Directing soft matter assembly for optimizing stimuli-response and*

properties" ACS National Meeting, Washington DC, August 2017

Bobby G. Sumpter, Invited Talk: "*Soft Matter Design through Guided Molecular Ordering*", 251st ACS National Meeting in San Diego, CA, March 2016.

Bobby G. Sumpter, "*Directing matter: From formation to function*", Clemson University, September 30, 2016.

Bobby G. Sumpter, Jacek Jakowski, Liangbo Liang, "*Sculpting at the Nanoscale"*, SERMACS, Columbia, SC October 2016.

Bobby G. Sumpter, "*Soft Matter is Hard but Ripe with Opportunities*", Physics Seminar, ORNL, March 10, 2016.

Jingsong Huang and Bobby G. Sumpter, "*Understanding Transport and Packing of Ionic Liquids during Electrode Charging*", 47th Central Regional Meeting of the American Chemical Society, Covington, KY, May 19, 2016.

Bobby G. Sumpter, "*ORNL Capabilities and Interests for Beyond Moore Computing*", Big Ideas Summit, Sandia National Labs, July 27-28, 2016

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

Bobby G. Sumpter, "*Untangling complexity in functional polymeric materials through integrated simulation, synthesis and neutron scattering*", Materials Research Society Meeting & Exposition, Boston, MA, December 3, 2015.

Bobby G. Sumpter, "*Untangling complexity in functional polymeric materials through integrated simulation, synthesis and neutron scattering*", Materials Research Society Meeting & Exposition, Boston, MA, December 3, 2015.

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, *Materials at Interfaces,* Frontiers in Data, Modeling and Simulation Workshop (invited), March 24, 2015, Argonne National Lab.

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, 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.

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