Bobby G. Sumpter

Section Head, Theory and Computation, Center for Nanophase Materials Sciences (CNMS), Oak Ridge National Laboratory

Oak Ridge National Laboratory
PO Box 2008
Oak Ridge, Tennessee 37831-6494

Phone: 865-574-4973
Email: sumpterbg@ornl.gov

Bobby G. Sumpter received his Bachelor of Science in chemistry from Southwestern Oklahoma State University (1983) and a doctorate 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 (1988–1992), Bobby joined the Chemistry Division at Oak Ridge National Laboratory in the Polymer Science group. He is currently the Deputy Director of the Center for Nanophase Materials Sciences, the group leader for the Computational Chemical and Materials Sciences, director/group leader of the Nanomaterials Theory Institute, and interim group leader for Macromolecular Nanomaterials at Oak Ridge National Laboratory. 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 multicomponent polymers and composites; confinement effects, and the physical, chemical, mechanical, and electronic properties of nanostructured materials. His research groups pursue forefront nanoscience using high-performance computing at scale and experimental synthesis/characterization.

EDUCATION

Oklahoma State University	PhD 1987 Physical Chemistry
Southwestern Oklahoma State University	BS 1983 Chemistry (ACS Certified)

GRADUATE AND POSTDOC ADVISORS

Graduate Advisor: Donald L. Thompson (University of Missouri, Columbia)

Postdoctoral Advisors: Greg S. Ezra (Cornell University), Bernhard Wunderlich (University of Tennessee, Oak Ridge National Laboratory)

PROFESSIONAL EXPERIENCE

2020-present PI of the "Closing the carbon cycle with data accelerated approaches" initiative at ORNL. Formulate, develop, communicate and direct the initiative.

2018-2020 Chair of the "Materials Innovation: From Atoms to Function" initiative at ORNL. Formulate and direct the initiative.

2017–present Chair ORNL Corporate Fellows Council. Engage with the ORNL leadership team and the corporate fellows in terms of ORNL strategies and talent management.

2018–2019 Interim Director, Center for Nanophase Materials Sciences (CNMS). This was from September 2018-January 2019. The role entailed taking care of all responsibilities for the successful operation, delivery of milestones, including those for the CNMS as a division in physical science directorate (similar to a department head).

2015–2020 Interim group leader for Macromolecular Nanomaterials, Center for Nanophase Materials Sciences (CNMS). Lead and coordinate the capabilities and research efforts of the group in polymer and soft matter; mentor the staff members toward successful careers.

2014–Present Deputy director, CNMS, Oak Ridge National Laboratory (ORNL). Coordinate scientific capabilities development and research directions for the CNMS. Mentor the staff members toward successful careers and the facility users toward successful project(s).

2013–Present Joint Faculty Professor, Bredesen Center for Interdisciplinary Research and Graduate Education, University of Tennessee (UT). Direct Ph.D. thesis research.

2013–Present ORNL Corporate Fellow. This is the highest scientific level of achievement at ORNL, recognizing outstanding accomplishments and leadership in science and the mission of ORNL.

2009–Present Group leader, Computational Chemical and Materials Sciences. Lead and coordinate the capability development and research efforts in computational sciences; mentor the staff members toward successful careers

2009–Present Director of the Nanomaterials Theory Institute, ORNL. Lead and coordinate the capability development and research efforts in nanomaterials theory; mentor the staff members toward successful careers.

2009–2013 Distinguished Research Staff, ORNL. This is a level for a staff member approximately similar to a full professor.

2006–2009 Senior Research Staff, CNMS, ORNL. The nanoscale science research centers came online in late 2005; became a senior staff member at CNMS.

2003–2009 Senior Research Staff, Computer Science and Mathematics Division (CSMD), ORNL. This is a level for a staff member approximately similar to an associate professor.

1992–2002 Research staff scientist, ORNL. This is a beginning level for a staff member at ORNL.

1988–1992 Research associate, UT/ORNL. A research position supporting work on polymer science projects joint between UT and ORNL at that time.

1987–1988 Postdoctoral research, Cornell University. Research in chemical physics and nonlinear dynamics

PROFESSIONAL ACTIVITIES, HONORS, AWARDS

Fellow American Physical Society (APS)

Fellow American Association for the Advancement of Sciences (AAAS)

Member American Physical Society, Materials Research Society (MRS), AAAS, American Chemical Society (ACS), American Ceramic Society (ACerS), International Neural Network Society (INNS), Association for Computing Machinery (ACM), Society of Engineering Science (SES), American Energy Society

Advisory Committees: Center for Predictive Simulation of Functional Materials (CPSFM), a DOE Computational Materials Sciences Center; Center for Molecular Design and Development (CMDD), at the University of Arkansas, Little Rock; Executive Committee for the Center for Understanding and Control of Acid Gas-induced Evolution of Materials for Energy (UNCAGE-ME) EFRC, Georgia Tech; Steering Committee Oak Ridge Institute (ORI) at UT; Science Alliance Advisory Board, University of Tennessee; Advisory board Biodesign Center for Sustainable Macromolecular Materials and Manufacturing (BCSM3) at Arizona State University (ASU)

2018-Present Chair of ORNL's Corporate Fellows Council

2015–2018 Vice chair ORNL Corporate Fellows Council

2014–Present Vice chair Corporate Fellows Scientific Advisory Council for the Computing and Computational Sciences Directorate (ORNL)

2014–Present Organization of ORNL Soft Matter Council

2018–2020 Materials Innovation Initiative Lead

2018 UT-Battelle award for Research Leadership, Group Level

2017 UT-Battelle award for Mentor of Early Career Staff

2017 CNMS Distinguished Scientific Paper

2017 CNMS Outstanding Scientific or Technical Contribution

2017 CNMS Distinguished Patent

2014 CNMS Distinguished Scientific Paper

2013 ORNL Corporate Fellow

2012 ORNL Significant Event Award

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 Chemical &Analytical Sciences Division Technical Achievement Award

JOURNAL EDITORIAL BOARDs (PRIOR)

Journal of Nanotechnology

International Journal of Smart Engineering System Design

BRIEF RESEARCH SYNOPSIS

Sumpter's 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. His work is closely coupled with experiments at the Center for Nanophase Materials Sciences and the Spallation Neutron Source, with a 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 innovations and improved materials for energy science and technology. Overall, this vision is aggressively pursued through a multipronged and tight integration with Oak Ridge National Laboratory's distinctive capabilities in precision experimental synthesis, state-of-the-art characterization, and leadership class computing.

Research Areas/Topics

1. **Computational Soft Condensed Matter Science.** The goal is to unravel the underlying multiscale physicochemical processes that control nanostructure morphologies and macroscopic physical, mechanical, electrical, and transport properties. In particular, the research seeks to understand how to design and control the nanoscale organization of macromolecular nanomaterials and their nanocomposites to achieve improved structure, properties, and functionality. This work highlights polymer-based materials for energy storage (supercapacitors and batteries), energy conversion (organic optoelectronics and photovoltaics), and lightweight structural materials (nanocomposites).
2. **Interfacial Mediated Interactions and Self-Assembly.** The goal is to understand the mechanisms 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. First-principles discovery and understanding enabled by high fidelity modeling/simulation are combined with unique experimental methods for producing materials with nanometer scale structure (synthesis, surface patterning, layer deposition, nanostructuring, etc.) and 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.** The goal is to understand how atomic scale structure, confinement, and quantum mechanical effects impact electronic processes within nanostructures and across interfaces. Very thin sheets of a material can exhibit greatly enhanced properties such as increased carrier mobility compared with the bulk and are well suited for applications in new electronic devices, super-strong lightweight composite materials, energy generation and storage. Focus is on reliably discovering and predicting structure-function-transport relationships.

4. **High-Capacity Energy Storage Materials.** The goal is to enable research that not only will lead to predictive simulations but also will advance the basic understanding of energy storage systems. Using theory, computational modeling, and simulation in direct corroboration with experiment, investigate electrochemical processes at the length and time scales where the underlying "behavior" is controlled. 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 insights 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 codesign materials and nanostructures to diminish degradation.

5. **Digital Twins for Materials Design, Characterization and Prediction.** The goal is to provide a computational-based capability using input from *in situ* and *ex situ* experimental tools like x-ray, neutron, scanning probes, chemical imaging, and high-resolution transmission electron microscopy; a first principles approach to enable rapid structural and dynamical characterization alongside predictive capabilities. This is a step toward multimodal, multiphysics fusion and deep data analytics enabled with machine learning. 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 and therefore theoretical and computational science when performed in concert with experiments can enable solving some of the grand challenges in energy science. ORNL's facilities and distinguishing capabilities provide a direct means to address this in terms of mathematics, computer science (leadership computing), and experimental imaging and characterization facilities.

PEER-REVIEWED JOURNAL PUBLICATIONS (H-INDEX = 75, ~24,500 CITATIONS GOOGLE SCHOLAR)

1. O. Dyck, M. Ziatdinov, S. Jesse, F. Bao, A.Y. Nobakht, A. Maksov, B.G. Sumpter, R. Archibald, K.J.H. Law, S.V. Kalinin, Probing potential energy landscape via electron-beam-induced single atom dynamics, *Acta Materialia* **203**, 116508 (2021).

2. V. Fung, G. Hu, P. Ganesh, B. G. Sumpter, Machine learned features from density of states for accurate adsorption energy prediction, *Nature Commun.* **12**, 1-11 (2021).

3. Guan-Rong Huang, Jan Michael Y Carrillo, Yangyang Wang, Changwoo Do, Lionel Porcar, Bobby G Sumpter, Wei-Ren Chen, An exact inversion method for extracting orientation ordering from small-angle scattering, *Phys. Chem. Chem. Phys*, (2021). DOI: 10.1039/D0CP05886F

4. Azhad U Chowdhury, Dongsook Chang, Yuewen Xu, Kunlun Hong, Bobby G Sumpter, Jan-Michael Y Carrillo, Benjamin Doughty, Mapping the interfacial chemistry and structure of partially fluorinated bottlebrush polymers and their linear analogues, *Langmuir*, **37**, 211-218 (2021).

5. X. Jiang, L. Sharma, V. Fung, S. J. Park, C.W. Jones, B.G. Sumpter, J. Baltrusaitis, Z. Wu, Oxidative dehydrogenation of propane and propylene with soft oxidants via heterogeneous catalysis, *ACS Catal.,* **11**, 2182−2234 (2021).

6. T. Yu, D. Lingerfelt, J. Jakowski, M.A. Jabed, P. Ganesh, B.G. Sumpter, Electron-beam-induced molecular plasmon excitation and energy transfer in silver molecular nanowires, *J. Phys. Chem. A* **125**, 1, 74–87 (2021).

7. Maxim Ziatdinov, Stephen Jesse, Bobby G Sumpter, Sergei V Kalinin, Ondrej Dyck, Tracking atomic structure evolution during directed electron beam induced Si-atom motion in graphene via dep machine learning, *Nanotech*. **32**, 035703 (2021).

8. David B Lingerfelt, Tao Yu, Anthony Yoshimura, Panchapakesan Ganesh, Jacek Jakowski, Bobby G Sumpter, Nonadiabatic effects on defect diffusion in silicon-doped nanographenes, *Nano. Lett.* **21**, 236-242 (2020).

9. Jyoti P Mahalik, Wei Li, Andrei T Savici, Steven Hahn, Hans Lauter, Haile Ambaye, Bobby G Sumpter, Valeria Lauter, Rajeev Kumar, Dispersity-driven stablization of coexisting morphologies in asymmetric diblock copolymer thin films, *Macromolecules,* **54,** 450-459 (2020).

10. Sheng Zhao, Yiman Zhang, Hoang Pham, Jan-Michael Y Carrillo, Bobby G Sumpter, Jagjit Nanda, Nancy J Dudney, Tomonori Saito, Alexei P Sokolov, Peng-Fei Cao, Improved single-ion conductivity of polymer electrolyte via accelerated segmental dynamics, *ACS Applied Energy Materials*, **12**, 1250-1258 (2020).

11. Kamal Choudhary, Kevin F Garrity, Andrew CE Reid, Brian DeCost, Adam J Biacchi, Angela R Hight Walker, Zachary Trautt, Jason Hattrick-Simpers, A Gilad Kusne, Andrea Centrone, Albert Davydov, Jie Jiang, Ruth Pachter, Gowoon Cheon, Evan Reed, Ankit Agrawal, Xiaofeng Qian, Vinit Sharma, Houlong Zhuang, Sergei V Kalinin, Bobby G Sumpter, Ghanshyam Pilania, Pinar Acar, Subhasish Mandal, Kristjan Haule, David Vanderbilt, Karin Rabe, Francesca Tavazza, The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design, *npj Computational Materials,* **6**, 173 (2020).

12. Wei Li, Jan-Michael Y Carrillo, Bobby G Sumpter, Rajeev Kumar, Modulating microphase separation of lamellae-forming diblock copolymers via ionic junctions, *ACS Macro Lett*., **11**, 1667-1673 (2020).

13. Ondrej Dyck, Cheng Zhang, Philip D. Rack, Jason D. Fowlkes, Bobby G. Sumpter, Andrew R. Lupini, Sergei V. Kalinin, Stephen Jesse, Electron-beam introduction of heteroatomic PtSi structures in graphene, *Carbon* **161**, 750-757 (2020).

14. David B. Lingerfelt, P. Ganesh, Jacek Jakowski, Bobby G. Sumpter, Understanding Beam Induced Electronic Excitations in Materials, *J. Chem. Theory Comput.* **16,** 1200-1214 (2020).

15. Daniel Salatto, Yuto T Koga, Yashasvi Bajaj, Zhixing Huang, Benjamin M Yavitt, Yizhi Meng, Jan-Michael Y Carrillo, Bobby G Sumpter, Dmytro Nykypanchuk, Takashi Taniguchi, Maya K Endoh, Tadanori Koga, Generalized protein-repellent properties of ultrathin homopolymer films, *Macromolecules* **53**, 6547-6554 (2020)

16. Rajeev Kumar, Jyoti P Mahalik, Kevin S Silmore, Zaneta Wojnarowska, Andrew Erwin, John F Ankner, Alexei P Sokolov, Bobby G Sumpter, Vera Bocharova, Capacitance of thin films containing polymerized ionic liquids, *Sci. Adv.*, **6** eaba7952 (2020).

17. Ali Yousefzadi Nobakht, Ondrej Dyck, David B Lingerfelt, Feng Bao, Maxim Ziatdinov, Artem Maksov, Bobby G Sumpter, Richard Archibald, Stephen Jesse, Sergei V Kalinin, Kody JH Law, Reconstruction of effective potential from statistical analysis of dynamic trajectories, *AIP Advances* **10**, 065034 (2020).

18. Xuanyu Zhang, Rui You, Zeyue Wei, Xiao Jiang, Jiuzhong Yang, Yang Pan, Peiwen Wu, Qingdong Jia, Zhenghong Bao, Lei Bai, Mingzhou Jin, Bobby Sumpter, Victor Fung, Weixin Huang, Zili Wu, Radical chemistry and reaction mechanisms of propane oxidative dehydrogenation over hexagonal boron nitride catalysts, *Angew. Chem.* **59**, 8042-8046 (2020).

19. Alison A Pawlicki, Dinesh G Bansal, Nikolay Borodinov, Alex Belianinov, Kerry Cogen, Dean Clarke, Bobby G Sumpter, Olga S Ovchinnikova, *In situ* multimodal imaging for nanoscale visualization of tribofilm formation, *J. Appl. Phys*. **15**, 154303 (2020).

20. Yongtao Liu, Anton V Ievlev, Liam Collins, Alex Belianinov, Jong K Keum, Mahshid Ahmadi, Stephen Jesse, Scott T Retterer, Kai Xiao, Jingsong Huang, Bobby G Sumpter, Sergei V Kalinin, Bin Hu, Olga S Ovchinnikova, Strain-chemical gradient and polarization in metal halide perovskites, *Adv. Electronic Materials* **6**, 1901235 (2020).

21. Vera Bocharova, Anne-Caroline Genix, Jan-Michael Y Carrillo, Rajeev Kumar, Bobby Carroll, Andrew Erwin, Dmitry Voylov, Alexander Kisliuk, Yangyang Wang, Bobby G Sumpter, Alexei P Sokolov, Addition of short polymer chains mechanically reinforces glassy poly(2-vinylpyridine)-silica nanoparticle nanocomposites, *ACS Appl. Nano. Materials* **3**, 3427-3438 (2020).

22. Victor Fung, Guoxiang Hu, Bobby Sumpter, Electronic band contraction induced low temperature methane activation on metal alloys, *J. Mat. Chem. A*. **8**, 6057-6066 (2020).

23. Jingjie Zhang, Xufan Li, Kai Xiao, Bobby G Sumpter, Avik W Ghosh, Liangbo Liang, The role of mid-gap phonon modes in thermal transport of transition metal dichalcogenides, *J. Phys. Cond. Matter* **32**, 025306 (2020).

24. Jenica Marie L Madridejos, Bálint Aradi, Bobby G Sumpter, Gregory F Metha, Stephan Irle, Density-functional tight-binding for phosphine-stabilized nanoscale gold clusters, *Chemical Science*, **11**, 13113-13128 (2020).

25. Alison A Pawlicki, Dinesh G Bansal, Nikolay Borodinov, Alex Belianinov, Kerry Cogen, Dean Clarke, Bobby G Sumpter, Olga S Ovchinnikova, *In situ* multimodal imaging for nanoscale visualization of tribofilm formation, *J. Appl. Phys*. **15**, 154303 (2020).

26. Dima Bolmatov, Jan-Michael Y. Carrillo, Bobby G. Sumpter, John Katsaras, Maxim O. Lavrentovich, Double membrane formation in heterogeneous vesicles, *Soft Matt*er **16**, 8806-8817 (2020).

27. Zihao Zhang, Jennifer A. Schott, Miaomiao Liu, Hao Chen, Xiuyang Lu, Bobby G. Sumpter, Sheng Dai, Prediction of carbon dioxide adsorption via deep learning, *Angewante Chemie*, **130**, 1-6 (2019).

28. Maxim Ziatdinov, Ondrej Dyck, Artem Maksov, Bobby G. Sumpter, Stephen Jesse, Rama K. Vasudevan, Sergei V. Kalinin, Building and exploring libraries of atomic defects in graphene: scanning transmission electron and scanning tunneling microscopy study, *Science Advances* **5**: eaaw8989 (2019).

29. J. Zhu, V.Q. Vuong, B.G. Sumpter, S. Irle, Artificial neural network correction for density-functional tight-binding molecular dynamics, *MRS Commun.* **9**, 867-873 (2019).

30. Artem Maksov, Ondrej Dyck, Kai Wang, David Geohegan, Bobby G. Sumpter, Rama Vasudevan, Stephen Jesse, Sergei Kalinin, Maxim Ziatdinov, Deep Learning Analysis of Defect and Phase Evolution During Electron Beam Induced Transformations in WS2, *NPJ Comp. Mat.* DOI:10.1038/s41524-019-0152-9 (2019).

31. D. Lingerfelt, J. Jakowski, P. Ganesh, B.G. Sumpter, Electronically nonadiabatic structural transformations promoted by electron beams, *Adv. Func. Mater*, 1901901 (2019).

32. X. Li, J. Zhang, A. A Puretzky, A. Yoshimura, X. Sang, Q. Cui, Y. Li, L. Liang, A. W Ghosh, H. Zhao, R. R Unocic, V. Meunier, C. M Rouleau, B. G Sumpter, D. B Geohegan, K. Xiao, Isotope-engineering the thermal conductivity of two-dimensional MoS_2, *ACS Nano* **13**, 2481-2489 (2019).

33. Yongtao Liu, Liam Collins, Roger Proksch, Songkil Kim, Brianna R. Watson, Benjamin Doughty, Tessa R. Calhoun, Mahshid Ahmadi, Anton V. Ievlev, Stephen Jesse, Scott T. Retterer, Alex Belianinov, Kai Xiao, Jingsong Huang, Bobby G. Sumpter, Sergei V. Kalinin, Bin Hu, Olga S. Ovchinnikova, Reply to "On the ferroelectricity of $CH_3NH_3PbI_3$ perovskites", *Nature Materials* **18**, 1051 (2019)

34. Yongtao Liu, Anton V. Ievlev, Liam Collins, Alex Belianinov, Jong K. Keum, Mahshid Ahmadi, Stephen Jesse, Scott T. Retterer, Kai Xiao, Jingsong Huang, Bobby G. Sumpter, Sergei V. Kalinin, Bin Hu, Olga S. Ovchinnikova, Light-ferroic interaction in hybrid organic inorganic perovskites, *Advanced Optical Materials* 1901451 (2019).

35. W.S. Xu, C.N. Lam, J-M. Carrillo, B.G. Sumpter, Y. Wang, Comment on "Relating chain conformations to extensional stress in entangled polymer melts", *Phys. Rev. Lett*. **122**, 059803 (2019).

36. Zhongcan Xiao, Chuanxu Ma, Wenchang Lu, Jingsong Huang, Liangbo Liang, Kunlun Hong, An-Ping Li, Bobby G. Sumpter, and Jerzy Bernholc, Ab initio investigation of the cyclodehydrogenation process for polyanthrylene transformation to graphene nanoribbons, *npj Computational Materials* **5:** 91 (2019).

37. Jie Fu, Sheng Dai, Ka Hung Lee, Udo Schnupf, Bobby G. Sumpter, Stephan Irle, Performance of DFTB in comparison to ab initio and first principles methods for isomer geometries and energies of glucose epimers in vacuo and solution, *ACS Omega* **3**, 16899-16915 (2019).

38. Dongsook Chang, Matthias Lorenz, Matthew J Burch, Olga S Ovchinnikova, Kunlun Hong, Bobby G Sumpter, Jan-Michael Y Carrillo, Structures of partially fluorinated bottlebrush polymers, *ACS Appl. Polymer Materials*, **2**, 209-219 (2019).

39. V.Q. Vuong, Y. Nishimot, D.G. Fedorovm B.G. Sumpter, T.A. Niehaus, S. Irle, The fragment molecular orbital method based on long-range corrected density functional tight-binding, *J. Chem. Theory & Comput.* **15**, 3008-3020 (2019).

40. W. Li, J-M. Carrillo, J. Katsaras, B.G. Sumpter, R. Ashkar, R. Kumar, The influence of curvature on domain distribution in binary mixture membranes, *Soft Matter* (2019). DOI: 10.1039/c9sm01262a

41. H. Lyu, C.J. Jafta, I. Popovs, H. Meyer, J.A Hachtel, J. Huang, B. G Sumpter, S. Dai, X-G.Sun, A dicyanobenzoquinone based cathode material for rechargeable lithium and sodium ion batteries, *J. Mat. Chem. A.* (2019). DOI: 10.1039/c9ta04869c

42. B. Doughty, A-C. Genix, I. Popov, B. Li, S. Zhao, T. Saito, D. A. Lutterman, R.L. Sacci, B. G. Sumpter, Z. Wojnarowska, V. Bocharova, Structural correlations tailor conductive properties in polymerized ionic liquids, *Phys. Chem. Chem. Phys*. **21**, 14775-14785 (2019).
43. Yuanhang Guo, Jieun Lee, Jinha Son, Suk-kyun Ahn, Jan-Michael Y Carrillo, Bobby G Sumpter, Decoding liquid crystal oligomer phase transitions: Toward molecularly engineered shape changing materials, *Macromoleculs* **52**, 6878-6888 (2019).

44. Chuanxu Ma, Zhongcan Xiao, Jingsong Huang, Liangbo Liang, Wenchang Lu, Kunlun Hong, Bobby G. Sumpter, J. Bernholc, An-Ping Li, Direct writing of heterostructures in single atomically precise graphene nanoribbons, *Phys. Rev. Mater.* **3**, 016001 (2019).

45. Eric S Muckley, Tolga Aytug, Richard Mayes, Andrew R Lupini, Jan-Michael Y Carrillo, Monojoy Goswami, Bobby G Sumpter, Ilia N Ivanov, Hierarchical TiO2:CuO Nanostructures for Gas/Vapor Sensing and CO2 Sequestration, *ACS Appl. Mat & Interfaces* **51**, 48466-48475 (2019).

46. Mohammed Alaboalirat, Kyle J. Arrington, Luqing Qi, Jong K. Keum, Jan-Michael Y. Carrillo, Bobby G. Sumpter, Rafael Verduzco, John Matson, Amphiphilic Bottlebrush Block Copolymers: Aqueous Self-Assembly Reveals Ultra-Low Critical Micelle Concentration, *Macromolecules* **52** 464-476 (2019).

47. Zhongcan Xiao, Chuanxu Ma, Jingsong Huang, Liangbo Liang, Wenchang Lu, Kunlun Hong, Bobby G. Sumpter, An-Ping Li,* and Jerzy Bernholc, Design of Atomically Precise Nanoscale Negative Differential Resistance Devices, *Adv. Theory Simul.* 1800172 (2019).

48. Jan-Michael Carrillo, Wei-Ren Chen, Zhe Wang, Bobby G. Sumpter, Yangyang Wang, Chain conformation of polymer melts with associating groups, *J. Phys. Commun.* **3**, 035007 (2019).

49. Tao Yu, Florence Fabunmi, Jingsong Huang, Bobby G. Sumpter, Jacek Jokowski, A fast scheme to calculate electronic couplings between P3HT polymer units using diabatic orbitals for charge transfer simulations, *J. Comp. Chem.* **40**, 532-542 (2019).

50. R. Kumar, W. Li, B.G. Sumpter, M. Muthukumar, Understanding the effects of dipolar interactions on the thermodynamics of diblock copolymer melts, *J. Chem. Phys.* **151**, 054902 (2019).

51. Dmitry Voylov, Vera Bocharova, Nickolay Lavrik, Ivan Vlassiouk, Georgios Polyzos, Alexei Volodin, Yury Shulga, Alexander Kisliuk, Thirumagal Thiyagarajan, Duane Miller, Ramesh Narayanan, Bobby Sumpter, Alexei Sokolov, Noncontact tip-enhanced Raman spectroscopy for nanomaterials and biomedical applications, *Nanoscale Advances*, **1**, 3392-3399 (2019).

52. Yuanghang Guo, Jieun Lee, Suk Kyun ahn, Jan Michael Carrillo, Bobby Sumpter, Decoding Liquid Crystal Oligomer Phase Transitions: Toward Molecularly Engineered Shape Changing Materials, *Macromolecules* **52**, 6879-6888 (2019).

53. Maya K Endoh, Yuma Morimitsu, Daniel Salatto, Zhixing Huang, Mani Sen, Weiyi Li, Yizhi Meng, David G Thanassi, Jan-Michael Y Carrillo, Bobby G Sumpter, Daisuke Kawaguchi, Keiji Tanaka, Tadanori Koga, Protein resistance driven by polymer nanostructure, *ACS Macro Letters* **8**, 1153-1159 (2019).

54. Maya Endoh, Yuma Morimitsu, Daniel Salatto, Zhixing Huang, Mani Sen, Weiyi Li, Yizhi Meng, David Thanassi, Jan Michael Carrillo, Bobby Sumpter, Daisuke Kawaguchi, Keiji Tanaka, Tadonori Koga, Protein Resistance Driven by Polymer Nanoarchitecture, *ACS Macro Letters* **8**, 1153-1159 (2019).

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56. T. Koga, D. Barkley, M. Nagao, T. Taniguchi, J-M. Carrillo, B.G. Sumpter, T. Masul, H. Kishimoto, M. Koga, J.G. Rudick, M.K. Endoh, Interphase Structures and Dynamics near Nanofiller Surfaces in Polymer Solutions, *Macromolecules* **51**, 9462-9470 (2018).

57. 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.* **4**: e1700336 (2018).

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59. Zhou Yu, Chao Fang, Jingsong Huang, Bobby G. Sumpter, Rui Qiao, Solvate ionic liquids at electrified interfaces, *ACS Applied Materials & Interfaces* **10**, 32151-32161 (2018).

60. Yongtao Liu, Liam Collins, Roger Proksch, Songkil Kim, Brianna R Watson, Benjamin Doughty, Tessa R Calhoun, Mahshid Ahmadi, Anton V Ievlev, Stephen Jesse, Scott T Retterer, Alex Belianinov, Kai Xiao, Jingsong Huang, Bobby G Sumpter, Sergei V Kalinin, Bin Hu, Olga S Ovchinnikova, Chemical nature of ferroelastic twin domains in $CH_3NH_3PbI_3$ perovskite, *Nature Materials* **17**, 1013–1019 (2018).

61. Yong-Hui Tian, Shuangli Hu, Xiaolan Sheng, Yixiang Duan, Jacek Jakowski, Bobby G. Sumpter, Jingsong Huang, Non-Transition Metal Catalytic System for N_2 Reduction to NH3: A DFT Study of Al-Doped Graphene, *J. Phys. Chem. Lett.* **9,** 570-576 (2018).

62. Wen-Sheng Xu, Christopher N Lam, Jan-Michael Y Carrillo, Bobby G Sumpter, Yangyang Wang, Comment on: "Relating Chain Conformations to Extensional Stress in Entangled Polymer Melts", *Phys. Rev. Lett.* **121**, 117801 (2018).

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1. US Patent Application 2009/0024,547, *Multi-Intelligent System for Toxicogenomic Applications (MISTA)*
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SELECTED RECENT INVITED TALKS (>200 CONTRIBUTED TALKS ARE NOT LISTED)

1. “*Computational Materials and Chemical Sciences: Part 1 and Part 2”* Cyber Training Summer School, June 2020.

2. "*Information Extraction, Analysis and Feedback for Directing Matter by Design,*" presentation was invited at APS and uploaded to the APS virtual on-line meeting for Data Science I. Big Data & ML. March 2020.

3. "*Understanding the Chemical and Materials World, Atom-by-Atom*" at the University of Tennessee, Knoxville, February 27, 2020.

4. "*Computational Materials Science*", RPI Computational Summer School, RPI July 2019.

5. "*Controlling Defects and Disorder in Low-Dimensional Materials*", IMRC, Cancun, August 2019.

6. "*Understanding and Tailoring Transport in Polymerized Ionic Liquids*", Santa Fe, September 2019.

7. *"Matching Theory, Simulation and Experiment Across Length and Time Scales for Accelerating Materials Discovery and Design*" at the Computational Materials Modeling Workshop, Virginia Tech, Blacksburg, VA, October 26, 2018.

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25. "*Theory-informed design of functional soft matter for energy science and technology"*, American Chemical Society National Meeting & Exposition, Boston, MA, August 19, (2015).

26. *"Polymers and Materials by Design"*, Duke University, September 18, (2015).

27. *"Materials at Interfaces",* Frontiers in Data, Modeling and Simulation Workshop, Argonne National Lab, March 24-2, (2015).

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

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

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

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

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

33. "*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).

34. "*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).

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

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

37. "*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).

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

39. "*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).

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

41. "*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).

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

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

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

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

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

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

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

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

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

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

52. "*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).

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

54. "*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).

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

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

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

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

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

60. "*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).

61. "*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).

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

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

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

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

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

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

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

69. "*Nanoscale Self-Assembly and Interfacial Interactions*", NSRCs Theory Workshop, Albuquerque, New Mexico, (2010).

70. "*Exploring Structure-Property Relationships in Nanoscale Graphitic Systems*", MRS International meeting, Cancun Mexico, August 2010.

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

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

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

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

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

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

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

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

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

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

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

82. "*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).

83. "*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).

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

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

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

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

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

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

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

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

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

93. "*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).

POSTDOCTORAL SCHOLARS MENTORED (RECENT)

Michael Drummond (now at University of North Texas)

De-en Jiang (now at University of California, Riverside)

Jingsong Huang (ORNL)

Alejandro Lopez-Benzanilla (now at Los Alamos National Laboratory)

Eduardo Cruz-Silva (now at GlobalFoundries)

Rajeev Kumar (ORNL)

Jan-Michael Carrillo (ORNL)

Jyoti Mahalik (now at U. Mass. Amherst)

RECENT FUNDING HISTORY

Multiple CRADA's, served as a theme leader at CNMS, led three groups with funding levels at ~9 M, helped sustain FWP's alongside facilitating bringing new ones to ORNL, theory effort on an EFRC, was the ORNL lead for a Mathematical Multifaceted Integrated Capability Centers (MMICCs), facilitated a new SciDAC and ECP projects, director of the NTI which coordinates upwards to 9M. Overall, my tenure at ORNL has consistently included full funding with a notable growth and support of 30+ staff, postdocs and students.

GRADUATE STUDENTS MENTORED (RECENT)

Served on the committees and/or co-advised 5 PhD 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, 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). Recent PhD graduate mentored, Artem Maksov (University of Tennessee in the Bredesen Center, 2019).

Summer Students/Interns. Through ORAU/ORISE/UTK continually mentored numerous summer students and visitors (>30).

REFERENCES

Prof. Vincent Meunier, Kodosky Constellation Chair Professor of Physics
Head, Physics Department, Rensselaer Polytechnic Institute, Troy, NY 12180
(meuniv@rpi.edu)

Prof. Robert J. Harrison, Department of Applied Mathematics & Statistics, Stony Brook University and Brookhaven National Lab, Director Institute for Advanced Computational Science, Stony Brook University, Stony Brook, NY 11794 (robert.harrison@stonybrook.edu)

Prof. Mauricio Terrones, Distinguished Professor of Physics, Chemistry and Materials Science & Engineering, Pennsylvania State University, University Park, PA 16802 (mtterrones@gmail.com or mut11@psu.edu)

Prof. Tom Russell, Department of Polymer Science and Engineering, University of Massachusetts, 120 Governors Drive, Amherst, MA 01003 (russell@mail.pse.umass.edu)

Prof. Jerry Bernholc, Department of Physics, North Carolina State University, Raleigh, NC 27695-8200 (bernholc@ncsu.edu)

Prof. Rui Qiao, John R. Jones III Faculty Fellow, Department of Mechanical Engineering, VirginialTech, Blacksburg, VA 24061 (ruiqiao@vt.edu)

Dr. Hans M. Christen, Director Neutron Scattering Division, Oak Ridge National Lab, Oak Ridge, TN 37831 (christenhm@ornl.gov)

Dr. Jeff Nichols, Associate Lab Director, Computing and Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831 (nicholsja@ornl.gov)