Bobby G. Sumpter

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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 Theory and Computation Section head at the Center for Nanophase Materials Sciences (CNMS). He previous served as the group leader for the Computational Chemical and Materials Sciences, director/group leader of the Nanomaterials Theory Institute, interim group leader for Macromolecular Nanomaterials, and the deputy director for CNMS 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, 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 with direct integration to experimental synthesis and 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 PI of the "Closing the carbon cycle with data accelerated approaches" initiative at ORNL. Formulate, develop, communicate, and direct the initiative.

2020-Present Theory and Computation Section Head, CNMS. Coordinate, hire, and plan the R&D strategy for two computational and data-centric groups in CNMS. Be a mentor for all staff members, postdocs, and students to ensure successful careers

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

2017–2022 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 and mentor the staff members toward successful careers.

2014–2021 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.

2009–2021 Group leader, Computational Chemical and Materials Sciences. Lead and coordinate the capability development and research efforts in computational sciences and mentor the staff members toward successful careers

2009–2021 Director of the Nanomaterials Theory Institute, ORNL. Lead and coordinate the capability development and research efforts in nanomaterials theory and 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)

Fellow Institute of Physics (IOP)

Fellow International Association of Advanced Materials (IAAM)

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)

2018-2022 Chair of ORNL's Corporate Fellows Council

2015–2018 Vice chair ORNL Corporate Fellows Council

2014–2020 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

Journal of Nanotechnology; International Journal of Smart Engineering System Design (prior)

Carbon Trends (Current)

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, multi-physics 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 = 89, ~33,500 CITATIONS GOOGLE SCHOLAR)

1. A. Fuhr, P. Ganesh, R.K. Vasudevan, K.M. Roccapriore, B.G. Sumpter, Digital twins and deep learning segmentation of defects in monolayer MX2 phases, *Appl. Phys. Lett.* **124**, 031901 (2024).

2. M. Flynn-Hepford, J. Lasseter, I. Kravchenko, S. Randolph, J. Keum, B.G. Sumpter, S. Jesse, P. Maksymovych, A. Talin, M. J. Marinella, P. D. Rack, A.V. Ievlev, O.S. Ovchinnikova, Direct Visualization of Charge Migration in Bilayer Tantalum Oxide Films by Multimodal Imaging, *Adv. Electron. Mater*. 10, 2300589 (2024).

3. P. Kumar, B.G. Sumpter, T. Saito, R.J. Davis Importance of hydrogen bonding in base-catalyzed transesterification reactions with vicinal diols, *Journal of Catalysis* **429**, 115246 (2024).

4. C-H. Tung, Y-J. Hsiao, H-L. Chen, G-R.Huang, L. Porcar, M-C. Chang, J-M. Carrillo, Y. Wang, B.G. Sumpter, Y. Shinohara, J. Taylor, C. Do, Wei-Ren Chen, Unveiling mesoscopic structures in distorted lamellar phases through deep learning-based small angle neutron scattering analysis, *Journal of Colloid and Interface Science* **659** 739 (2024).

5. J. Tang, S. Li, D. Wang, Q. Zheng, J. Zhang, T. Lu, J. Yu, L. Sun, B. Sa, B.G. Sumpter, J. Huang, W. Sun, Enriching 2D transition metal borides via MB XMenes (M = Fe, Co, Ir): Strong correlation and magnetism, *Nanoscale Horizons*, **9**, 162 (2024).

6. C-H. Tung, S-Y. Chang, S. Yip, Y. Wang, J-M. Carrillo, B.G. Sumpter, Y. Shinohara, C. Do, W-R. Chen, Viscoelastic relaxation and topological fluctuations in glass forming liquids, *J. Chem. Phys*, **160**, 094506 (2024).

7. N. Kanbargi, J.T. Damron, Y. Gao, L.T. Kearney, J-M. Carrillo, J.K. Keum, B.G. Sumpter, A. K. Naskar, Amplifying Nanoparticle Reinforcement through Low Volume Topologically Controlled Chemical Coupling, *ACS Macro. Lett*. **13**, 280 (2024).

8. B.G. Sumpter, V. Meunier, Digital twins in materials and chemical sciences, *Carbon Trends*, **13**, 100297 (2023).

9. A. Fuhr, B.G. Sumpter, P. Ganesh, Defects go green: using defects in nanomaterials for renewable energy and environmental sustainability, *Front. Nanotechnol*. **5**, (2023).

10. J-M. Carrillo, Y. Wang, R. Kumar, B.G. Sumpter, Coarse-grained explicit-solvent molecular dynamics simulations of semidilute unentangled polyelectrolyte solutions, *Eur. Phys. J. E* **46**:92 (2023).

11. O. Popova, S.J. Randolph, S.M. Neumayer, L. Liang, B. Lawrie, O.S. Ovchinnikova, R. J. Bondi, M.J. Marinellla, B.G. Sumpter, P. Maksymovych, Nanoscale imaging of He-ion irradiation effects on amorphous toward electroforming-free neuromorphic functions, *Appl. Phys. Lett.* **123**, 153503 (2023).

12. N. Sivadas, B.G. Sumpter, P. Ganesh, Scale-free switching of polarization in the layered ferroelectric material CuInP2S6, *Phys. Rev. Res*. **5**, 043074 (2023).

13. Unsupervised Machine Learning Discovery of Chemical and Physical Transformation Pathways from Imaging Data, *APL Machine Learning* **1**, 026117 (2023).

14. Local conformations and heterogeneities in structures and dynamics of isotactic polypropylene adsorbed onto carbon fiber, *Polymer* **256**, 125584 (2023).

15. Autonomous continuous flow reactor synthesis for scalable atom-precision, *Carbon Trends*, **10**, 100234 (2023).

16. Machine Intelligence-Centered System for Automated Characterization of Functional Materials and Interfaces, *ACS Applied Materials & Interfaces* **15**, 2329–2340 (2023). **[Highlight]**

17. Abisko: Deep codesign of an architecture for spiking neural networks using novel neuromorphic materials, *The International Journal of High Performance Computing Applications*, **37**(3-4) 351–379 (2023). **[Highlight]**

18. Selective deconstruction of mixed plastics by a tailored organocatalyst, *Materials Horizons* **10**, 3360-3368 (2023). **[Front cover of journal and Highlight]**

19. Chemical upcycling of polyethylene, polypropylene, and mixtures to high-value surfactants, *Science* **381,** 666-671 (2023). **[Highlight]**

20. Mechanisms Controlling the Energy Barrier for Ion Hopping in Polymer Electrolytes, *Macromolecules* **6**, 6051–6059 (2023).

21. Anti-polyelectrolyte and polyelectrolyte effects on conformations of polyzwitterionic chains in dilute aqueous solutions, *PNAS Nexus* **2**, 1-10 (2023). **[Highlight]**

22. The Role of SnO2 Processing on Ionic Distribution in Double-Cation–Double Halide Perovskites, *ACS Applied Materials & Interfaces* **15**, 36856–36865 (2023).

23. A Graph Dynamical neural network approach for decoding dynamical states in ferroelectrics, *Carbon Trends* **11**, 100264 (2023).

24. Inferring colloidal interaction from scattering by machine learning, *Carbon Trends* **10**, 100252 (2023).

25. Double-Atom Catalysts Featuring Inverse Sandwich Structure for CO2 Reduction Reaction: A Synergetic First-Principles and Machine Learning Investigation, *ACS Catalysis* **13,** 9616–9628 (2023). **[Front cover of Journal]**

26. Structure-Based Design of Dual Bactericidal and Bacteria-Releasing Nanosurfaces, *ACS Applied Materials & Interfaces* **5**, 3420–3432 (2023).

27. Assembly of polyelectrolyte star block copolymers at the oil–water interface, *Nanoscale* **15**, 1042-1052 (2023). **[Back cover of journal and Highlight]**

28. Understanding Interfacial Block Copolymer Structure and Dynamics, *Macromolecules* 56, 762–771 (2023). **[Highlight]**

29. Extracting Inelastic Scattering Cross Sections for Finite and Aperiodic Materials from Electronic Dynamics Simulations, *J. Chem Theory and Computation* **18**, 7093–7107 (2023). **[Front Cover of Journal]**
30. A Novel Dynamic Polymer Synthesis via Chlorinated Solvent Quenched Depolymerization, *CCS Chemistry* **5**, 1841-1853 (2023).

31. Strain-Induced asymmetry and on-site dynamics of silicon defects in graphene, *Carbon Trends* **9**, 100189 (2022).

32. Quantum theory of electronic excitation and sputtering by transmission electron microscopy, *Nanoscale* **15**, 1053-1067 (2023).

33. Can a Deep-learning Model make Fast Predictions of Vacancy Formation in Diverse Materials? *AIP Advances* **13**, 095109 (2023).

34. Mesoscopic two-point collective dynamics of glass-forming liquids, *J. Chem. Phys.* **159**, 114501 (2023). **[Editors choice]**

35. Coarse-Grained Explicit-Solvent Molecular Dynamics Simulations of Semidilute Unentangled Polyelectrolyte Solutions*, The European Physical Journal E.* 46, 92 (2023).

36. Scale-free switching of polarization in the layered ferroelectric material CuInP 2S6, *Phys. Rev. Res*. (2023).

37. Strain-Induced asymmetry and on-site dynamics of silicon defects in graphene, *Carbon Trends*, **9**, 100189 (2022).

38. Fingerprinting Brownian Motions of Polymers, *Physical Review Letters* **129**, 057801 (2022).

39. Dynamic aspects of graphene deformation and fracture from approximate density functional theory, *Carbon* **190** 183-193 (2022).

40. Physically Informed Machine Learning Prediction of Electronic Density of States, *Chemistry of Materials* **34,** 4848–4855 (2022).

41. Understanding the Impacts of Support−Polymer Interactions on the Dynamics of Poly(ethyleneimine) Confined in Mesoporous SBA-15*, J. Amer. Chem. Soc.* **144**, 11664–11675 (2022).

42. Deep Generative Models for Materials Discovery and Machine Learning-Accelerated Innovation, *Front. Mater*. **9**, 865270 (2022).

43. Quantum theory of electronic excitation and sputtering by transmission electron microscopy, *Nanoscale* DOI: **10.1039/D2NR01018F** (2022).

44. Learning in continuous action space for developing high dimensional potential energy models, *Nature Comm,* **13**, 368 (2022).

45. A machine learning inversion scheme for determining interaction from scattering, *Nature Comm. Phys.* **5**, 46 (2022).

46. Bridging microscopy with molecular dynamics and quantum simulations: an atomAI based pipeline, *npj Comp. Mater.* **8**, 74 (2022).

47. The Local Topological Free Energy of the SARS-CoV-2 Spike Protein, *Polymers* **14**, 3014 (2022).

48. Decoding polymer self-dynamics using a two-step approach, *Phys. Rev. E.* **106**, 014502 (2022).

49. Small angle scattering of diblock copolymers profiled by machine learning, *J. Chem. Phys.* **156**, 131101 (2022).

50. CO2-Assisted Oxidative Dehydrogenation of Propane over VOx/In2O3 Catalysts: Interplay between Redox Property and Acid-Base Interaction, *ACS Catalysis* **12**, 11239-11252 (2022).

51. Highly Fluorescent Purine-Containing Conjugated Copolymers with Tailored Optoelectronic Properties, *Polymer Chemistry* **13**, 4921-4933 (2022).

52. A Novel Dynamic Polymer Synthesis via Chlorinated Solvent Quenched Depolymerization, *CCS Chemistry*, (2022). DOI: 10.31635/ccschem.022.202202362

53. Extracting Inelastic Scattering Cross Sections for Finite and Aperiodic Materials from Electronic Dynamics Simulations, *JCTC* (2022). DOI: 10.1021/acs.jctc.2c00882

54. Quantum theory of electronic excitation and sputtering by transmission electron microscopy, *Nanoscale* DOI: **10.1039/D2NR01018F** (2022).

55. Topological Effects Near Order−Disorder Transitions in Symmetric Diblock Copolymer Melts *Macromolecules* **54**, 7492–7499 (2021). DOI: 10.1021/acs.macromol.1c00780 (2021).

56. Single-atom catalysts with anionic metal centers: Promising electrocatalysts for the oxygen reduction reaction and beyond*, J. Energy Chem,* **63** 285–293 (2021).

57. Structural and Dynamical Roles of Bound Polymer Chains in Rubber Reinforcement, *Macromolecules* **54**, 11032–11046 (2021).

58. Inverse design of two-dimensional materials with invertible neural networks*, npj Comp. Mater*. **7**, 200 (2021).

59. Spatial Correlations of Entangled Polymer Dynamics, *Phys. Rev. E.* **104**, 024503 (2021).

60. 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).

61. Kevin M Roccapriore, Qiang Zou, Lizhi Zhang, Rui Xue, Jiaqiang Yan, Maxim Ziatdinov, Mingming Fu, David G Mandrus, Mina Yoon, Bobby G Sumpter, Zheng Gai, Sergei V Kalinin, Revealing the Chemical Bonding in Adatom Arrays via Machine Learning of Hyperspectral Scanning Tunneling Spectroscopy Data, *ACS Nano* **15**, 11806-11816 (2021).

62. 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).

63. Ayana Ghosh, Bobby G Sumpter, Ondrej Dyck, Sergei V Kalinin, Maxim Ziatdinov, Ensemble learning-iterative training machine learning for uncertainty quantification and automated experiment in atom-resolved microscopy, *npj Comp. Mater*. **7**: 100 (2021).

64. 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).

65. 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).

66. Si Luo, Meijun Li, Victor Fung, Bobby G Sumpter, Jue Liu, Zili Wu, Katharine Page, New Insights into the Bulk and Surface Defect Structures of Ceria Nanocrystals from Neutron Scattering Study, *Chem. Mater*. **33**, 3959-3970 (2021).

67. 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).

68. On-surface cyclodehydrogenation reaction pathway determined by selective molecular deuterations, *Chemical Science* **12**, 15637-15644 (2021).

69. Jinxing Gu, Ziyuan Zhao, Jingsong Huang, Bobby G Sumpter, Zhongfang Chen, MX Anti-MXenes from Non-van der Waals Bulks for Electrochemical Applications: The Merit of Metallicity and Active Basal Plane, *ACS Nano* **15**, 6233-6242 (2021).

70. Jyoti P. Mahalik, Wei Li, Andrei T. Savici, Steven Hahn, Hans Lauter, Haile Ambaye, Bobby G. Sumpter,Valeria Lauter, Rajeev Kumar, Dispersity Driven Stabilization of Coexisting Morphologies in Asymmetric Diblock Copolymer Thin Films, *Macromolecules* **54**, 450–459 (2021).

71. Gernot Rother, Uma Tumuluri, Kuan Huang, William T. Heller, Sheng Dai, Jan-Michael Carrillo, Bobby G. Sumpter, Interactions of imine polymer with nanoporous silica and carbon in hybrid adsorbents for carbon capture, *Langmuir*, **37**, 4622–4631 (2021).

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

73. Yongtao Liu, Bobby G. Sumpter, Jong K. Keum, Bin Hu, Mahshid Ahmadi, Olga S. Ovchinnikova, Strain in Metal Halide Perovskites: The Critical Role of A-Site Cation, *ACS Applied Energy Materials* **4**, 2068–2072 (2021).

74. Sergei V. Kalinin, Maxim Ziatdinov, Jacob Hinkle, Stephen Jesse, Ayana Ghosh, Kyle P. Kelley, Andrew R. Lupini, Bobby G. Sumpter, and Rama K. Vasudevan, Automated and Autonomous Experiments in Electron and Scanning Probe Microscopy, *ACS Nano* **15**, 12604-12627 (2021).

75. V. Fung, J. Zhang, E. Juarez, B.G. Sumpter, Benchmarking graph neural networks for materials chemistry, *npj Comp. Mater.* **7**:84 (2021)

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77. Guan-Rong Huang, Jan Michael Carrillo, Yangyang Wang, Changwoo Do, Lionel Porcar, Bobby Sumpter, Wei-Ren Chen, An exact inversion method for extracting orientation ordering by small-angle scattering, *Phys. Chem. Chem. Phys.* **23**, 4120-4132 (2021).

78. Sheng Zhao, Yiman Zhang, Hoang Pham, Jan-Michael Y. Carrillo, Bobby G. Sumpter, Jagit Nanda, Nancy Dudney, Tomonori Saito, Alexei P. Sokolov, Peng-Fei Ca, Improved Single-ion Conductivity of Polymer Electrolyte via Accelerated Segmental Dynamics, *ACS Applied Energy Materials*, **3**, 12540–12548 (2020).

79. 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).

80. 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 Comp. Mater.,* **6**, 173 (2020).

81. 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).

82. 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).

83. 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).

84. 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)

85. 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).

86. 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).

87. 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).

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2. 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).

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4. David Lingerfelt, Panchapakesan Ganesh, Bobby G. Sumpter, Jacek Jakowski, From Ground to Excited Electronic State Dynamics of Electron and Ion Irradiated Graphene Nanomaterials, Chapter 8, Elsevier (2021).

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US Patent 10,777,381 “*Beam Controlled Nano-robotic Device*”, October 2020.

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PATENTS PENDING

1. US Patent Application 2009/0024,547, *Multi-Intelligent System for Toxicogenomic Applications (MISTA)*
2. US Patent Application 12/758,930, *Olefin-Containing Fuel Composition and Method*

>300 INVITED AND CONTRIBUTED TALKS

POSTDOCTORAL SCHOLARS MENTORED (RECENT)

Michael Drummond (now at University of North Texas)

De-en Jiang (now at Vanderbilt University)

Jingsong Huang (now at ORNL)

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

Eduardo Cruz-Silva (now at GlobalFoundries)

Rajeev Kumar (now at ORNL)

Jan-Michael Carrillo (now at ORNL)

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).