Bobby G. Sumpter

Director
Nanomaterials Theory Institute
Center For Nanophase Materials Sciences Division
Group Leader Computational Chemical and Materials Sciences
Computer Science & Mathematics Division
Oak Ridge National Laboratory (ORNL)
(865) 574-4973
sumpterbg@ornl.gov

Education

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

Professional Experience

2009-present	Group Leader, Computational Chemical and Materials Sciences and Director of the Nanomaterials Theory Institute, ORNL
2009–present	Distinguished Research Staff
2006–2009	Senior Research Staff, Center for Nanophase Materials Sciences, ORNL
2003–2009	Senior Research Staff, Computer Science & Mathematics Division, ORNL
1992–2002	Research staff scientist, ORNL
1988–1992	Research Associate, UT/ORNL
1987–1988	Postdoctoral Research, Cornell University

Honors and Awards

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

Professional Membership

American Physical Society (APS)
American Chemical Society (ACS)
Materials Research Society (MRS)
American Association for the Advancement in Science (AAAS)
International Neural Network Society (INNS)

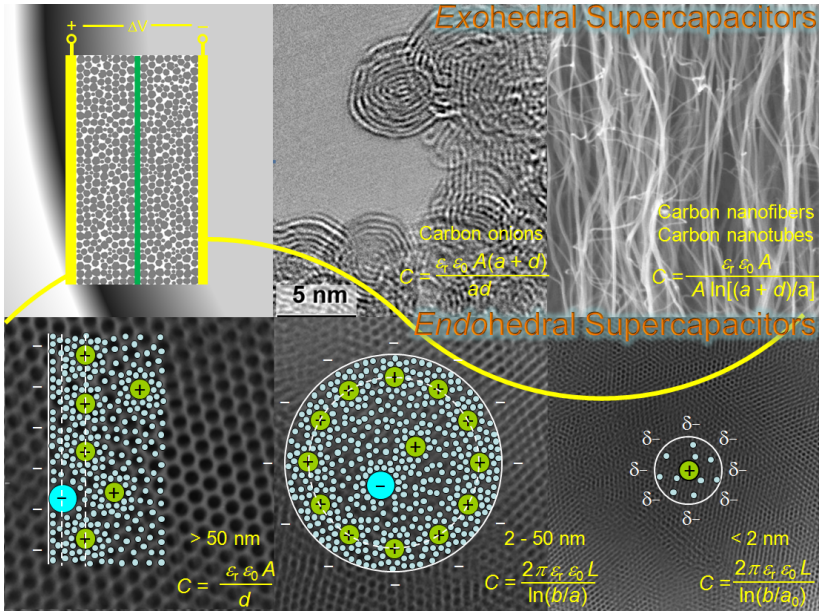
Journal Editorial Board

Journal of Nanotechnology
International Journal of Smart Engineering System Design

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 1986. Following postdoctoral studies in Chemical Physics at Cornell University 1987-1988 and in Polymer Chemistry at the University of Tennessee, Bobby joined the Chemistry Division at Oak Ridge National Laboratory in the Polymer Science group. He is currently the group leader for the Computational Chemical and Materials Sciences group and the Nanomaterials Theory Institute. Dr Sumpters' research is focused on the fundamental understanding of nanoscale self-assembly processes, interactions at interfaces, the structure and dynamics of molecular-based materials including multi-component polymers and composites, and the physical, mechanical and electronic properties of nanostructured materials.

Brief Research Synopsis

My research is directed primarily toward developing and applying modern computational and mathematical capabilities for the understanding and prediction of chemical and physical processes ranging from the molecular to the nanoscale to full-size engineering applications, using a multidisplinary approach that integrates chemistry, physics, materials science, mechanical engineering, and biology. Work is closely coupled with the Nanomaterials Theory Institute at the Center for Nanophase Materials Sciences, where scientific focus is 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. This vision is possible through a multi-pronged, holistic, and tight integration with Oak Ridge National Labortory distinctive capabilities in precision experimental synthesis and characterization along side leadership class computing.



Research Areas/Topics:

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

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

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

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

(5) **"Virtual" Materials Characterization/Prediction**: A computational-based capability using input from on-line experimental tools like X-ray, neutron, HTEM, scanning probes, various spectroscopies, and a purely first principles

approach, to enable rapid structural and dynamical characterization: A step towards multi-instrument, multi-physics fusion. The thesis for this work is that structure and properties of molecules, solids, and liquids are direct reflections of the underlying quantum motion of their electrons, theoretical and computational science when performed in concert with experiments offers great opportunity toward helping solve some of the grand challenges in energy science. Modern facilities provide a direct means to address this capability, in terms of mathematics (MMICCs), computer science (leadership computing), and best-in-class experimental characterization facilities.

Peer Reviewed Journal Publications: overall h-index 39 (ISI), 44 (Google Scholar), >5000 citations
1-250

1. Eduardo Cruz-Silva, Xiaoting Jia, Humberto Terrones, Bobby G. Sumpter, Mauricio Terrones, Mildred S. Dresselhaus, Vincent Meunier, Edge-edge interactions in stacked graphene nanoplatelets, *ACS Nano.* **7**, 2834–2841 (2013) dx.doi.org 10.1021/nn4004204.
2. C. Dyer, P. Driva, S. Sides, B. G. Sumpter, J. Mays, J. Chen, R. Kumar, M. Goswami, M. Dadmun, Effect of Macromolecular Architecture on the Morphology of Polystyrene–Polyisoprene Block Copolymers, *Macromolecules* **46**, 2023–2031 (2013) dx.doi.org/10.1021/ma202650a.
3. Kai Xiao, Wan Deng, Jong Keum, Mina Yoon, Ivan V. Vlassiouk, Kendal W. Clark, An-Ping Li, Ivan I. Kravchenko, Gong Gu, Andrew Payzant, Bobby G. Sumpter, Sean Smith, Jim Browning, David B. Geohegan. Surface-Induced Orientation Control of CuPc Molecules for the Epitaxial Growth of Highly Ordered Organic Crystals on Graphene, *J. Am. Chem. Soc.* **135**, 3680-3687 (2013) dx.doi.org/10.1021 /ja3125096.
4. Josue Ortiz-Medina, M. Luisa García-Betancourt, Xiaoting Jia, Rafael Martínez-Gordillo, Miguel A. Pelagio-Flores, David Swanson, Ana Laura Elías, Humberto R. Gutiérrez, Eduardo Gracia-Espino, Vincent Meunier, Jonathan Owens, Bobby G. Sumpter, Eduardo Cruz-Silva, Fernando J. Rodríguez-Macías, Florentino López-Urías, Emilio Muñoz-Sandoval, Mildred S. Dresselhaus, Humberto Terrones,Mauricio Terrones, Nitrogen-Doped Graphitic Nanoribbons: Synthesis, Characterization and Transport, *Adv. Func. Mater.* DOI: 10.1002/adfm.201202947 (2013).
5. K. R. S. Chandrakumar, Alex A. Puretzky, Chris Rouleau, Jason Readle, David B. Geohegan, Karren More, Gerd Duscher, Bobby Sumpter, Stephan Irle, Keiji Morokuma, High-temperature transformation of Fe-decorated single-wall carbon nanohorns to nanooysters: a combined experimental and theoretical study, *Nanoscale* **5**, 1849-1857 (2013).
6. K. Misichronis, S. Rangou, E. Ashcraft, R. Kumar, M. Dadmun, B.G. Sumpter, J. W. Mays, N. E. Zafeiropoulos , A. Avgeropoulos, Synthesis, Characterization (Molecular-Morphological) and Theoretical Morphology

Predictions of Poly(cyclohexadiene) Containing Linear Triblock Terpolymers, *Polymer* **54**, 1480-1489 (2013) dx.doi.org/10.1016/j.polymer.2013.01.005.

7. Rajeev Kumar, Scott W. Sides, Monojoy Goswami, Bobby G. Sumpter, Kunlun Hong, Konstantinos Misichronis, Apostolos Avgeropoulos, Thodoris Tsoukatos, Nikos Hadjichristidis, Frederick L. Beyer, Jimmy W. Mays, Morphologies of ABC tri-block terpolymer melts containing poly(cyclohexadiene): effects of conformational asymmetry, *Langmuir* **29**, 1995–2006 (2013) dx.doi.org/10.1021/la304576c.
8. Rajeev Kumar, Monojoy Goswami, Bobby G. Sumpter, Vladimir N. Novikov, Alexei P. Sokolov, Effects of backbone rigidity on the local structure and dynamics in polymer melts and glasses, *Phys. Chem. Chem. Phys.* **15**, 4604-4609 (2013) DOI: 10.1039/c3cp43737j.
9. Pan Zhu, Bobby G. Sumpter, Vincent Meunier, Electronic, Thermal and Structural Properties of Graphene Oxide Frameworks, *J. Phys. Chem. C.* **17** 8276–8281 (2013).
10. Qing Li, Jonathan R. Owens, Chengbo Han, Bobby G. Sumpter, Wenchang Lu, Jerry Bernholc, V. Meunier, Petro Maksymovych, Miguel Fuentes-Cabrera, Minghu Pan, Self-Organized and Cu-Coordinated Surface Linear Polymerization, ***Nature Scientific Reports*** *(~accepted)*.
11. Alejandro Lopez-Bezanilla, P. Ganesh, P. R. C. Kent, and Bobby G. Sumpter, Spin-Resolved Self-Doping Tunes the Intrinsic Half-Metallicity of AlN Nanoribbons, *Nano Research* (under review).
12. Jihua Chen, Ming Shao, Kai Xiao, Adam J. Rondinone, Yueh-Lin Loo, John E. Anthony, Paul R. C. Kent, Bobby G. Sumpter, Jingsong Huang, Solvent-Type-Dependent Crystalline Polymorphism of High Performance, Small Molecule Organic Semiconductor Thin Films Fabricated by Slow Solution Crystallization, *Nano Lett.,* under review (2013).
13. Alejandro Lopez-Bezanilla, Jingsong Huang, Paul R. C. Kent, Bobby G. Sumpter, Tuning From Half-Metallic to Semiconducting Behavior in SiC Nanoribbons, *Small* under review (2013).
14. Geoffrey A. Rojas, P. Ganesh, Simon J. Kelly, Bobby G. Sumpter, John A. Schlueter, Petro Maksymovych, Ionic Decomposition of Charge Transfer Salts Driven by Surface Epitaxy, *J. Phys. Chem. C. (*under review*)*.
15. Takuya Hayashi, Thomas C. O'Connor, Katsuhisa Higashiyama, Kohei Nishi, Tomohiro Tojo, Hiroyuki Muramatsu, Yoong Ahm Kim, Bobby G. Sumpter, Vincent Meunier, Mauricio Terrones, Morinobu Endo, A reversible strain-induced electrical conductivity in cup-stacked carbon nanotubes, ***Nanoscale*** (*accepted*).
16. J. Campos-Delgado, D.L. Baptista, M. Fuentes-Cabrera, B.G. Sumpter, V. Menier, H. Terrones, Y.A. Kim, H. Muramatsu, T. Hayashi, M. Endo, M. Terrones"Iron particle nano-drilling of few layer graphene at low electron beam accelerating voltages", *Particle* **30**, 76-82 (2013).
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20. A. Lopez-Bezanilla, J. Campos-Delgado, B. G. Sumpter, D.L. Baptista, T. Hayashi, Y.A. Kim, H. Muramatsu, M. Endo, C.A. Achete, M. Terrones, V. Meunier, Geometric and Electronic Structure of Closed Graphene Edges, *J. Phys. Chem. Lett*. **3**, 2097 (2012).
21. Wang, X., Goswami, M., Kumar, R., Sumpter, B. G. & Mays, J. Morphologies of block copolymers composed of charged and neutral blocks. *Soft Matter* **8**, 3036-3052, doi:10.1039/c2sm07223h (2012).
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29. Jakowski, J., Irle, S., Sumpter, B. G. & Morokuma, K. Modeling Charge Transfer in Fullerene Collisions via Real-Time Electron Dynamics. *Journal of Physical Chemistry Letters* **3**, 1536-1542, doi:10.1021/jz3004377 (2012).
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35. Wu, P., Huang, J., Meunier, V., Sumpter, B. G. & Qiao, R. Complex Capacitance Scaling in Ionic Liquids-Filled Nanopores. *Acs Nano* **5**, 9044-9051, doi:10.1021/nn203260w (2011).
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43. Lopez-Bezanilla, A., Huang, J., Terrones, H. & Sumpter, B. G. Boron Nitride Nanoribbons Become Metallic. *Nano Letters* **11**, 3267-3273, doi:10.1021/nl201616h (2011).
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Tautomerization, Magnetism, and Thermochromism. *Chemistry of Materials* **23**, 874-885, doi:10.1021/cm102320b (2011).
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251-273

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1. 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).
2. 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).
3. E. C Gira, L. Liang, J. Owens, E. Cruz-Silva, B. G. Sumpter, V. Meunier, "Electronic Transport in Graphitic Carbon Nanoribbons", Wiley (2012).
4. 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).
5. 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).
6. Vincent Meunier, Bobby G. Sumpter, "Carbon Nanotube Memory Elements", in Handbook of Nanophysics, CRC Press ISBN: 978-1-4200-7550-2 (2010).
7. 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).
8. 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).
9. 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).
10. 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).

11. 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).
12. 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).
13. "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).
14. "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).
15. "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).
16. "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).
17. 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).
18. 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).
19. 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).
20. 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).
21. Coral Getino, Jesus Santamaria, Jerry A. Darsey and Bobby G. Sumpter, "Conformational Energy and Molecular Dynamics Studies of the Conducting Polymer Poly(Phenylenevinylene)", in *Computer Simulation of Polymers*, Chapter 2, pp 15-40 (1990).

Patents

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

Patents pending

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

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

Active Invention Disclosures

#201202834: Electron-Induced Tautomerization for Patterning of Organic Molecules on Solid Surfaces

Invited talks over last 5 years: ~8/yr invited, 10/yr contributed (not listed)

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).

"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).

"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).

"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)

Workshop/Conference Organization and Session Chair over Last 3 years

Session chair, "Recent Advances in Materials Physics Symposium", NCSU, Raleigh, NC May (2012).

Session Chair for oral session 12.3 “Computational Physics and Sustainable Energy”, Conference on Computational Physics 2011, Gatlingburg, TN Oct. 30- Nov. 3 (2011).

2011 ASCR/BES Data Workshop: Chair for the section on “Theory and Algorithms”, Bethesda, Oct. 24-25 (2011).

Session chair, “Recent Advances in Materials Physics Symposium”, NCSU, Raleigh, NC May (2012).

Workshop**: “**Theory and Simulation of Nano Scale Materials”, Albuquerque, New Mexico, Oct. 14-15 (2010).

“1st Joint Workshop on Large-Scale Computer Simulation”, Aachen Germany, March (2011).

“Collaborative Workshop on Bio-catalysis”, Denver, CO, May 26 (2011).

Workshop: “Materials by Design”, Oak Ridge, TN Sep. 21-22 (2011).

Workshop: “Sustainable Energy Future: Nanomaterials Enabled Photovoltaics”, Oak Ridge, TN Sep. 22-23 (2011).

Session Chair March 2009, ACS National Meeting (Salt Lake, UT).

Session Chair and Scientific Committee, September 2009, ICAM09.

Session Chair and Co-organizer, August 2008, IEEE Nano (Dallas,TX)

Session Chair, APS March meeting 2010 (Portland, OR).

Workshop on Computation modeling and Neutron Science, Argonne (2010)

CNMS Workshop on “Next Generation Force Fields for Nanoscience” (2010)

DoE NSRC workshop for theoretical nanoscience (2010)

Collaborations During Past Five Years: Mike Barnes, Tom Russell– University of Massachuseets Amherst; Steven Stuart, Rui Qiao – Clemson University; 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– TechX Corporation; Ed Valeev – Virginia Tech; J. Leszczynski – Jackson State University; David Keefer, Mark Dadmun, Jimmy Mays – University of Tennessee; Martin Bakker – University of Alabama; Ian Gould – Imperial College London, M.S. Dresselhaus – MIT; M. Terrones – IPICYT; 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–RPI; Mauricio Terrnones – Penn. State; P.M. Ajayan – Rice

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

Postdoctoral Scholars Mentored (recent): Michael Drummond, De-en Jiang, Jingsong Huang, Monojoy Goswami, Edurado Cruz-Silva, Rajeev Kumar, Alejandro Lopez-Benzanilla

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).

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