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Publications

Education

Georgetown University, Washington, DC	Physical Chemistry	Ph.D. 2006
Nankai University, Tianjin, China	Physical Chemistry	M.S. 1994
Southwest University, Chongqing, China	Chemistry	B.S. 1991

Professional Experience

2023–p	Senior R&D Staff, ORNL
2015–2023	R&D Staff, ORNL
2010–2014	R&D Associate, ORNL
2007–2010	Postdoctoral Research Associate, ORAU/ORNL
2006–2007	Research Fellow, Chemistry Department, Georgetown University
1999–2006	Teaching/Research Assistant, Chemistry Department, Georgetown University
1994–1999	Engineer, Southwest R&D Institute of Chemical Industry, Chengdu, China

Service

2008–p	PSD Strategic Planning – Working Group for Strategy Development in CO_2 capture, conversion, and removal (2022); CNMS NERSC PI proxy for allocation and proposal renewals; CNMS/CSED Postdoc Hiring Committees; reviewer for SEED proposal and PTS/RESolution; International conferences panel discussion and session chair
2006–p	Associate Editor for Frontiers in Soft Matter (accepted invitation in Sep 2022 of Roberto Ricciardi, Head of Editor Outreach at Frontiers); Reviewer for proposals of NSF and ACS PRF; Reviewer including adjudicating reviewer for various journals of American Chemical Society (ACS), American Physical Society (APS), Chinese Academy of Sciences (CAS), Elsevier, Institute of Physics (IOP), Nature Publishing Group (NPG), Royal Society of Chemistry (RSC), Springer, Wiley-VCH, and World Scientific

Award

2019	Director's Award for Team Accomplishment in Science and Technology, UT-Battelle Awards Night, ORNL
2019	Team Award for Research Accomplishment in Science and Technology, UT-Battelle Awards Night, ORNL
2015	Distinguished Award for a Scientific or Technical Contribution, CSMD, ORNL
2012	Distinguished Scientific Paper Published, CSMD, ORNL
2008	IBM-Löwdin Fellowship, the 48th Sanibel Symposium
2006	Harold N. Glassman Dissertation Award in Sciences, Graduate School of Arts and Sciences, Georgetown University

Short Bio

My initial background was experimental organic chemistry and physical chemistry, with some experiences in chemical industry. I pivoted to theoretical and computational studies of physical and chemical problems of functional materials in 1999. Research expertise lies mainly in the modeling/simulation/theory of structure-property correlation, weak covalent bonding interactions, and electrical energy conversion/storage, by development of theoretical models and by application of various levels of theory such as CCSD(T), QCISD(T), DFT, time-dependent DFT, EPT, quasiparticle GW, ACFDT-RPA, and BSE. With a background of an experimental chemist and expertise of a theoretical and computational chemist, my primary goal is to bridge experimental observations with theoretical insights, thereby lending support to material discovery and optimization.

Research Areas/Topics

1. *Structure-property correlations of organic, inorganic, and hybrid materials* of 0D through 3D (molecular, polymeric, layered, and bulk materials). Examples of organic materials are conjugated polymers, molecular crystals of pentacene derivatives, anthradithiophene derivatives, BTQBT, and graphene nanoribbons, while examples of inorganic materials include graphene, SiC, hBN, MXenes, XMenes, TMDs, and Cd (or Zn) chalcogenides, and examples of hybrid materials are polyoxometalates and $CH_3NH_3PbI_3$. These materials are important for applications in electronic devices such as light-emitting diodes, photovoltaics, field effect transistors, magnetooptics, spintropics, etc. Main structural property is the crystal packing. The calculations of electronic properties include crystal orbitals, band structures, density of states, COOP, charge carrier properties, intermolecular transfer integrals, and various physical properties such as thermochromism, photochromism, solid-state UV-Vis, fundamental and optical band gaps, angle-resolved photoelectron spectroscopy (ARPES) as a function of both $k_{//}$ and $k_{\perp}$, electron affinity, ionization potential, and work function of surfaces and edges. We are also interested in charge and spin density wave phenomena.
2. *Unusual multicenter covalent π–π bonding interactions* of long distance (~3Å) between organic π-radicals or biradicaloids. Typical examples are phenalenyl and spiro-biphenalenyl monoradical and biradical derivatives, and TTF-TCNQ which are exploited as the building blocks for organic metals. "Pancake" bonds are predicted for electron- and hole-doped graphene bilayers as well. Some of these materials form organic conductors due to the electron delocalizations – thus giving organic metal without metal elements. Some others display magnetic properties due to the electron localizations. The conducting pathway along the π–π stacking and the magnetic exchanges between neighboring unpaired spins are deeply rooted in the novel multicenter covalent π–π bondings. Since chemical bonds usually go hand in hand with magnetism, we study the weak π–π bonding using magnetic properties measured by ESR, Faraday balance, or SQUID. Specifically, we conduct broken symmetry or spin-polarized DFT calculations and then compare with the analysis of experimental data with different models such as the alternating chain models, the Bleaney-Bowers dimer model, and extended Bleaney-Bowers dimer models. The weak bonding interactions may render an alteration of electrical, optical, or magnetic properties by the change of external stimuli, and thus giving rise to "smart materials".
3. *Electrical energy conversion/storage* with supercapacitors, Li- and Na-ion batteries, Li-S batteries, solid-state proton exchange electrolytes, electrochemical evolution of H_2, and electrochemical reduction of O_2, N_2, and CO_2. This fits especially well the US DOE's mission of discovering new materials for energy conversion/storage. For supercapacitors, we pay special attention to the electric double layer structure at the interface of porous carbon and various electrolytes (aqueous, organic, and ionic liquid). For Li-S batteries, we scrutinize the reaction mechanism on the S cathode without additive and with additive that serves as the catalyst to promote the dissolution of solid Li_2S deposits. Molecular dynamics is instrumental in clarifying the reaction mechanism of the electrochemical reaction at the interface. Additionally, we perform rational design of solid-state proton exchange electrolytes for Li^+ conduction. We are particularly interested in electrochemical reduction of the inert and refractory N_2 and CO_2 by using the ultrastrong electric field created by sharp carbon nanospikes at the electric double layer. Reaction mechanisms are also studied for thermal catalysis on single-atom catalysts and coinage metal substrates.

Peer Reviewed Journal Publications (*corresponding authors)

1. 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 Horiz.* **9**, 162-173 (2024).
2. J. Jakowski*, J. Huang, S. Z. Islam, D. S. Sholl, "Quantum Chemical Simulations of CO_2 and N_2 Capture in Reline, a Prototypical Deep Eutectic Solvent", *J. Phys. Chem. B* **127**, 8888-8899 (2023).
3. S. Islam*, Md Arifuzzaman, G. Rother, V. Bocharova, R. Sacci, J. Jakowski, J. Huang, I. Ivanov, R. Bhave*, T. Saito, D. Sholl, "A Membrane Contactor Enabling Energy-Efficient CO_2 capture from Point Sources with Deep Eutectic Solvents", *Ind. Eng. Chem. Res.* **62**, 4455-4465 (2023).

4. L. Yu, F. Li*, J. Huang*, B. G. Sumpter, W. E. Mustain, Z. Chen*, "Double-Atom Catalysts Featuring Inverse Sandwich Structure for CO_2 Reduction Reaction: A Synergetic First-Principles and Machine Learning Investigation", *ACS Catal.* 13, 9616-9628 (2022).
5. S. Garashchuk, J. Huang, B. G. Sumpter, J. Jakowski*, "From Classical to Quantum Dynamics of Atomic and Ionic Species Interacting with Graphene and Its Analogue", *Theor. Comput. Chem.* **21**, 61-86 (2022).
6. C. Ma, Z. Xiao, P. V. Bonnesen, L. Liang, A. A. Puretzky, J. Huang*, M. Kolmer, B. G. Sumpter, W. Lu, K. Hong, J. Bernholc, A.-P. Li*, "On-Surface Cyclodehydrogenation Reaction Pathway Determined by Selective Molecular Deuterations", *Chem. Sci.* **12**, 15637-15644 (2021).
7. J. Gu, Y. Zhao, S. Lin, J. Huang*, C. R. Cabrera, B. G. Sumpter, Z. Chen*, "Single-Atom Catalysts with Anionic Metal Centers: Promising Electrocatalysts for Oxygen Reduction Reaction and Beyond," *J. Energy Chem.* **63**, 285-293 (2021).
8. J. Gu, Z. Zhao, J. Huang*, B. G. Sumpter, Z. 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).
9. G. Hu*, V. Fung, J. Huang, P. Ganesh*, "Work Function Engineering of 2D Materials: The role of Polar Edge Reconstructions," *J. Phys. Chem. Lett.* **12**, 2320-2326 (2021).
10. Q. Gao, W. Sun*, P. Ilani-Kashkouli, A. Tselev, P. R. C. Kent, N. Kabengi, M. Naguib, M. Alhabeb, A. P. Baddorf, J. Huang, S. Jesse, Y. Gogotsi, N. Balke*, "Tracking Ion Intercalation into Layered Ti_3C_2 MXene Films across Length Scales," *Energy Environ. Sci.* **13**, 2549-2558 (2020).
11. C. Ma, Z. Xiao, A. A. Puretzsky, H. Wang, A. Mohsin, J. Huang, L. Liang, Y. Luo, B. J. Lawrie, G. Gu, W. Lu, K. Hong, J. Bernholc, A.-P. Li*, "Engineering Edge States of Graphene Nanoribbons for Narrow-Band Photoluminescence," *ACS Nano* **14**, 5090-5098 (2020).
12. Y. Liu, A. V. Ievlev, L. Collins, A. Belianinov, J. K. Keum, M. Ahmadi, S. Jesse, S. T. Retterer, K. Xiao, J. Huang, B. G. Sumpter, S. V. Kalinin, B. Hu, and O. S. Ovchinnikova*, "Strain-Chemical Gradient and Polarization in Metal Halide Perovskites," *Adv. Electron. Mater.* **6**, 1901235 (2020).
13. C. Ma, Z. Xiao, W. Lu, J. Huang, K. Hong, J. Bernholc, A.-P. Li*, "Step Edge-Mediated Assembly of Periodic Arrays of Long Graphene Nanoribbons on Au(111)," *Chem. Commun.* **55**, 11848-11851 (2019).
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15. Z. Xiao, C. Ma, W. Lu, J. Huang, L. Liang, A. Li, B. G. Sumpter, J. Bernholc*, "Ab Initio Investigation of the Cyclodehydrogenation Process for Polyanthrylene Transformation to Graphene Nanoribbons," *npj Comput. Mater.* **5**, 91 (2019).
16. J. A. Hachtel*, J. Huang, I. Popovs, S. Jansone-Popova, J. K. Keum, J. Jakowski, T. C. Lovejoy, N. Dellby, O. L. Krivanek, J. C. Idrobo*, "Identification of Site-Specific Isotopic Labels by Vibrational Spectroscopy in the Electron Microscope," *Science* **363**, 525-528 (2019).
17. Z. Xiao, C. Ma, J. Huang, L. Liang, W. Lu, K. Hong, B. G. Sumpter, A.-P. Li*, J. Bernholc*, "Design of Atomically Precise Nanoscale Negative Differential Resistance Devices," *Adv. Theory Simul.* **2**, 1800172 (2019).
18. T. Yu*, F. Fabunmi, J. Huang, B. G. Sumpter, J. Jakowski*, "A Fast Scheme to Calculate Electronic Couplings between P3HT Polymer Units Using Diabatic Orbitals for Charge Transfer Dynamics Simulations," *J. Comput. Chem.* **40**, 532-542 (2019).
19. C. Ma, Z. Xiao, J. Huang, L. Liang, W. Lu, K. Hong, B. G. Sumpter, J. Bernholc*, A.-P. Li*, "Direct Writing of Heterostructures in Single Atomically Precise Graphene Nanoribbons," *Phys. Rev. Mater.* **3**, 016001 (2019).
20. H. Lyu, C. J. Jafta, I. Popovs, H. M. Meyer, J. A. Hachtel, J. Huang*, B. G. Sumpter, D. Dai, X.-G. Sun*, "A Dicyanobenzoquinone Based Cathode Material for Rechargeable Lithium and Sodium Ion Batteries," *J. Mater. Chem. A* **7**, 17888-17895 (2019).
21. A. J. Rondinone*, J. Huang*, "Geometry Aids Green Carbon Electrochemistry," *Nat. Catal.* **1**, 903-904 (2018).

22. D. Chang*, T. Li, L. Li, J. Jakowski, J. Huang, J. K. Keum, B. Lee, P. V. Bonnesen, M. Zhou, S. Garashchuk, B. G. Sumpter, K. Hong*, "Selectively Deuterated Poly(ε-caprolactone)s: Synthesis and Isotope Effects on the Crystal Structures and Properties," *Macromolecules* **51**, 9393-9404 (2018).
23. F. Zhang, Z. Yu, A. J. Rondinone, J. Huang, B. G. Sumpter, R. Qiao*, "Adsorption of Molecular Nitrogen in Electrical Double Layers near Planar and Atomically Sharp Electrodes," *Langmuir* **34**, 14552-14561 (2018).
24. J. Jakowski*, J. Huang, B. G. Sumpter, S. Garashchuk*, "Theoretical Assessment of the Nuclear Quantum Effects on Polymer Crystallinity via Perturbation Theory and Dynamic," *Int. J. Quantum Chem.* **118**, e25712 (2018).
25. Z. Yu, C. Fang, J. Huang, B. G. Sumpter, R. Qiao*, "Molecular Structure and Dynamics of Interfacial Polymerized Ionic Liquids," *J. Phys. Chem. C* **122**, 22494-22503 (2018).
26. Z. Yu, C. Fang, J. Huang*, B. G. Sumpter, R. Qiao*, "Solvate Ionic Liquids at Electrified Interfaces," *ACS Appl. Mater. Interfaces* **10**, 32151-32161 (2018).
27. Y. Liu, L. Collins, R. Proksch, S. Kim, B. R. Watson, B. Doughty, T. R. Calhoun, M. Ahmadi, A. V. Ievlev, S. Jesse, S. T. Retterer, A. Belianinov, K. Xiao, J. Huang, B. G. Sumpter, S. V. Kalinin, B. Hu, O. S. Ovchinnikova*, "Chemical Nature of Ferroelastic Twin Domains in $CH_3NH_3PbI_3$ Perovskite," *Nat. Mater.* **17**, 1013-1019 (2018).
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29. C. Hu, J. Huang, B. G. Sumpter, E. Meletis, T. Dumitrica*, "Ab Initio Predictions of Strong Interfaces in Transition-Metal Carbides and Nitrides for Superhard Nano-Composite Coating Applications," *ACS Appl. Nano Mater.* **1**, 2029-2035 (2018).
30. Y.-H. Tian*, S. Hu, X. Sheng, B. G. Sumpter, J. Huang, "Non-Transition-Metal Catalytic System for N_2 Reduction to NH_3: A DFT Study of Al-Doped Graphene," *J. Phys. Chem. Lett.* **9**, 570-576 (2018).
31. C. Hu, P. Ni, L. Zhan, H. Zhao, J. He*, T. M. Tritt, J. Huang*, B. G. Sumpter, "Theoretical Investigations of Electrical Transport Properties in $CoSb_3$ Skutterudites under Hydrostatic Loadings," *Rare Met.* **37**, 316-325 (2018).
32. C. Hu, J. Huang, B. G. Sumpter, E. I. Meletis, T. Dumitrica*, "Ab Initio Predictions of Hexagonal Zr(B,C,N) Polymorphs for Coherent Interface Design," *J. Phys. Chem. C* **121**, 26007-26018 (2017).
33. N. Ekanayake, J. Huang, J. Jakowski, B. G. Sumpter, S. Garashchuk*, "Relevance of the Nuclear Quantum Effects on the Proton/Deuteron Transmission through Hexagonal Boron Nitride and Graphene Monolayers," *J. Phys. Chem. C* **121**, 24335-24344 (2017).
34. Z. Yu, F. Zhang, J. Huang, B. G. Sumpter, R. Qiao*, "Ionic Liquids-Mediated Interactions between Nanorods*," J. Chem. Phys.* **147**, 134704 (2017).
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36. B. Yang, C. Brown, J. Huang, L. Collins, X. Sang, R. R. Unocic, S. Jesse, S. V. Kalinlin, A. Belianinov, D. B. Geohagan, B. G. Sumpter, K. Xiao, O. S. Ovchinnikova*, "Enhancing Ion Migration in Grain Boundaries of Hybrid Organic-Inorganic Perovskites by Chlorine," *Adv. Funct. Mater.* **27**, 1700749 (2017).
37. W. Cui, S. Xu, B. Yan, Q. Xu*, B. G. Sumpter, J. Huang, S. Yin, H.-J. Zhao, Y. Wang*, "Triphasic 2D Materials by Vertically Stacking Laterally Heterostructured 2H-/1T'-MoS_2 on Graphene for Enhanced Photoresponse," *Adv. Electron. Mater.* **3**, 1700024 (2017).
38. F. Zhang, Y. He, J. Huang, B. G. Sumpter, R. Qiao*, "Multicomponent Gas Storage in Organic Cage Molecules," *J. Phys. Chem. C* **121**, 12426-12433 (2017).
39. C. Hu, X. Zeng, Y. Liu, M. Zhou, H. Zhao, T. M. Tritt, J. He*, J. Jakowski, P. R. C. Kent, J. Huang*, B. G. Sumpter, "Effects of Partial La Filling and Sb Vacancy Defects on $CoSb_3$ Skutterudites," *Phys. Rev. B* **95**, 155204 (2017).
40. C. Ma, Z. Xiao, H. Zhang, L. Liang, J. Huang, B. G. Sumpter, W. Lu, K. Hong, J. Bernholc, A.-P. Li*, "Controllable Conversion of Quasi-Freestanding Polymer Chains to Graphene Nanoribbons," *Nat. Commun.* **8**, 14815 (2017).

41. J. Lee, J. Huang, B. G. Sumpter, M. Yoon*, "Strain-Engineered Optoelectronic Properties of 2D Transition Metal Dichalcogenide Lateral Heterostructures," *2D Mater.* **4**, 021016 (2017).
42. T. S. Humble*, M. N. Ericson, J. Jakowski, J. Huang, C. Britton, F. G. Curtis, E. F. Dumitrescu, F. A. Mohiyaddin, B. G. Sumpter, "A Computational Workflow for Designing Silicon Donor Qubits," *Nanotechnology* **27**, 424002 (2016).
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45. Y. Tian*, J. Huang, X. Sheng, B. G. Sumpter, M. Yoon, M. Kertesz, "Nitrogen Doping Enables Covalent-Like $\pi-\pi$ Bonding between Graphenes," *Nano Lett.* **15**, 5482-5491 (2015).
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91. J. Huang*, F. Yao, J. Wei, Z. Zhou, W. Hu, "Hydrogen Diffusion in Amorphous $Ti_{0.88}Ni_{1.00}$ Film," *Chin. Chem. Lett.* **8**, 1005-1006 (1997).
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Book Chapters

97. S. Garashchuk, J. Huang, B. G. Sumpter, J. Jakowski*, "From Classical to Quantum Dynamics of Atomic and Ionic Species Interacting with Graphene and Its Analogue," in "Properties and Functionalization of Graphene: A Computational Chemistry Approach", Elsevier, 2020 – Invited contribution.
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Conference Proceedings

102. J. A. Hachtel*, J. Huang, I. Popovs, S. Jansone-Popova, J. K. Keum, J. Jakowski, T. C. Lovejoy, N. Dellby, O. L. Krivanek, J. C. Idrobo, "Damage-Free Nanoscale Isotopic Analysis of Biological Materials with Vibrational Electron Spectroscopy," *Microsc. Microanal.* **25(S2)**, 1088-1089 (2019).
103. A. Lopez-Bezanilla*, J. Huang, H. Terrones, B. G. Sumpter, "Electronic Structure Calculations on Edge-Functionalized Armchair Boron Nitride Nanoribbons," DOE's Science Discovery through Advanced Computing (SciDAC), published online (2011).
104. V. Meunier*, J. Huang, G. Feng, R. Qiao, B. G. Sumpter, "Modern Theories of Carbon-Based Electrochemical Capacitors: A Short Review," ASME International Mechanical Engineering Congress & Exposition, Paper Number: IMECE2010-41003 (2010).
105. G. Feng, R. Qiao, J. Huang, B. G. Sumpter, V. Meunier*, "Computational Modeling of Carbon Nanostructures for Energy Storage Applications," Proceeding of the 2010 10th IEEE Conference on Nanotechnology, NANO 2010, Article number 5698075, pp 100-104 (2010).
106. J. Huang*, B. G. Sumpter, V. Meunier, "Capacitor Models for Various Regimes, Carbons, and Electrolytes," Proceedings of the 2009 Advanced Automotive Battery and Capacitor Conference (AABC-09), Long Beach, CA. (2009).

Invited Talks (selected recent)

1. Theoretical Studies of Functional Materials for Photochromic, Thermochromic, and Electrochemical Applications, The 8th N.I.C.E. International Conference on Bio-inspiration, keynote talk invited by Frederic Guittard, Jun 20-22 (2023).
2. Theoretical Modeling and Computations of New Materials for Electrochemical Energy Conversion/Storage Devices, The Seventh Edition of Global Energy Meet (GEM-2023), invited by Conference Organizer, Mar 06-08 (2023).
3. Carbon Nanostructures for Energy Conversion and Storage: From Li-S Battery, Supercapacitors, to Nitrogen Fixation, 2022 TechConnect World Innovation Conference, invited by Christopher Sims, Wolfgang Bacsa, and Dalia Yablon, Jun 13-15 (2022).
4. The Effects of Ultrastrong Electric Field on Electroreduction of N_2 to NH_3 – A Theoretical Understanding, 2021 Joint Nanoscience and Neutron Scattering User Meeting Workshop, invited by Ilia N. Ivanov and Christopher Tulk, August 9-12 (2021).
5. Net-Zero Carbon Fuel Research, ORNL Net-Zero Carbon Workshop for Transportation, National Transportation Research Center, Knoxville, TN, invited by Michelle Kidder, January 31 (2019).

Graduate and Postdoctoral Advisors

Prof. Miklos Kertesz
Dr. Vincent Meunier and Dr. Bobby G. Sumpter

Postdoctoral Scholar Advised

Dr. Jia Zhou

Graduate Students Advised

Lili Qiu (summer intern, Georgetown University)
Chongze Hu (summer intern, University of Minnesota Twin Cities)

Undergraduate Students Advised

Chongze Hu (summer intern, Clemson University)
Dillon G. Gagnon (DOE SULI program, Purdue University Fort Wayne)
Ian J. Bongalonta (DOE SULI program, Clemson University; co-advised with Dr. Jacek Jakowski)
Nicholas L. Saunders (DOE SULI program, University of Dayton)
Chuck Moody (DOE CCI Program, Pellissippi State Community College)

High School Students Advised
Anna Y. Duke (thesis research, Farragut High School)
Peter Ni (service to ORNL, Montgomery High School)