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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

2015–p	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 started to embark on theoretical and computational studies of physical and chemical problems of functional materials from 1999. Research experiences are mainly 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 establish the bridge between experimental observations and theoretical rationalizations, which will hopefully lend supports for material discovery and experimental 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 Publications Metrics

1. Total citations = ~6650 (Google Scholar)
2. H-index = 37 and i10-index = 69 (Google Scholar)
3. Total publications = ~100 (listed below)
4. Total 40 as (co-)corresponding and as first or last if not (co-)corresponding author$^{\blacklozenge}$
5. Total 17 works sent to US DOE as highlights†; total 7 works in ORNL press release‡
6. ACS Editors' choice article = $1^{\Diamond}$; article frontispiece = 2^{Δ}; journal cover = 3^{∇}

Peer Reviewed Journal Publications (*corresponding authors)

1. J. Huang*, P. Ganesh, B. G. Sumpter, D. S. Sholl, K. Hong, "Interpreting Binary Azeotropes Based on A Theoretical Model Generalized from Raoult's Law and Henry's Law", uploaded to

ChemRxiv, to be divided into two manuscripts and submitted to *J. Chem. Educ.* (2022).♦

2. D. G. Gagnon, A. Y. Duke, P. Doak, J. Jakowski, I. N. Ivanov, A. J. Rondinone, S. T. Retterer, P. Ganesh, B. G. Sumpter, J. Huang*, "Activation of Nitrogen under Ultrastrong Electric Fields toward One-Electron Attachment", to be polished and submitted to *J. Chem. Phys.* (2022).♦
3. J. A. Hachtel*, J. Jakowski, J. Huang, S. Jansone-Popova, I. Popovs, E. A. Richardson, B. R. Evans, P. Rez, E. V. Formo*, "A New Path to Nanoscale Cellular Analysis with Monochromated Electron Energy-Loss Spectroscopy", uploaded to *arXiv*, currently under review *PNAS USA* (2022).
4. 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", under review *Ind. Eng. Chem. Res.* (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).♦†◊ [Tweeted by Prof. Yury Gogotsi https://twitter.com/gogotsi1/status/1372626769073819659.]
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).‡ [ORNL press release at https://www.ornl.gov/news/faster-more-efficient-energy-storage-could-stem-holistic-study-layered-materials.]
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).
14. 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, and O. S. Ovchinnikova*, "Reply to 'On the Ferroelectricity of $CH_3NH_3PbI_3$ Perovskites'", *Nat. Mater.* **18**, 1051-1053 (2019).
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).†‡ [ORNL press release at https://www.ornl.gov/news/novel-electron-microscopy-offers-nanoscale-damage-free-tracking-isotopes-amino-acids.]
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).†‡ [ORNL press release at https://www.ornl.gov/news/multimodal-imaging-shows-strain-can-drive-chemistry-photovoltaic-material?page=1]
28. Y. Song, D. Johnson, R. Peng, D. K. Hensley, P. V. Bonnesen, L. Liang, J. Huang, F. Yang, F. Zhang, R. Qiao, A. P. Baddorf, T. Tschaplinski, N. L. Engle, M. C. Hatzell, 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," *Sci. Adv.* **4**, e1700336 (2018).‡ [Invited to give a soundbite in ORNL press release at https://www.ornl.gov/news/novel-reaction-could-spark-alternate-approach-ammonia-production.]
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).
35. J. Jakowski*, J. Huang, S. Garashchuk, K. Hong, J. Keum, B. G. Sumpter, "Deuteration as a Means to Tune Crystallinity of Conducting Polymers," *J. Phys. Chem. Lett.* **8**, 4333-4340 (2017).

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).†‡Δ [ORNL press release at https://www.ornl.gov/news/imaging-ionic-moves.]
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).†‡ [ORNL press release at https://www.ornl. gov/news/built-bottom-nanoribbons-pave-way-states-graphene.]
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).
43. F. Zhang, F. Yang, J. Huang, B. G. Sumpter, R. Qiao*, "Thermodynamics and Kinetics of Gas Storage in Porous Liquids," *J. Phys. Chem. B* **120**, 7195-7200 (2016).
44. Y. He, R. Qiao*, J. Vatamanu, O. Borodin, D. Bedrov, J. Huang, B. G. Sumpter, "The Importance of Ion Packing on the Dynamics of Ionic Liquids during Micropore Charging," *J. Phys. Chem. Lett.* **7**, 36-42 (2016).
45. Y. Tian*, J. Huang, X. Sheng, B. G. Sumpter, M. Yoon, M. Kertesz, "Nitrogen Doping Enables Covalent-Like π–π Bonding between Graphenes," *Nano Lett.* **15**, 5482-5491 (2015).†
46. Y. Liu, C. Z. Hu, J. Huang, B. G. Sumpter, R. Qiao*, "Tuning Interfacial Thermal Conductance of Graphene Embedded in Soft Materials by Vacancy Defects," *J. Chem. Phys.* **142**, 244703 (2015).
47. Y. Tian*, B. G. Sumpter, S. Du, J. Huang*, "Pancake π–π Bonding Goes Double: Unexpected 4e/All-Sites Bonding in Boron- and Nitrogen-Doped Phenalenyls," *J. Phys. Chem. Lett.* **6**, 2318-2325 (2015).♦
48. Y. Bai, H.-M. He, Y. Li, Z.-R. Li*, Z.-J. Zhou, J.-J. Wang, D. Wu, W. Chen, F.-L. Gu*, B. G. Sumpter, J. Huang*, "Electric Field Effects on the Intermolecular Interactions in Water Whiskers: Insight from Structures, Energetics, and Properties," *J. Phys. Chem. A* **119**, 2083-2090 (2015).♦
49. J. Zhou*, B. G. Sumpter, P. R. C. Kent, J. Huang, "A Novel and Functional Single-Layer Sheet of ZnSe," *ACS Appl. Mater. Interfaces* **7**, 1458-1464 (2015).♦†
50. Y. Wang, B. G. Sumpter, J. Huang*, H. Zhang, P. Liu, H. Yang, H. Zhao*, "Density Functional Studies of Stoichiometric Surfaces of Orthorhombic Hybrid Perovskite $CH_3NH_3PbI_3$," *J. Phys. Chem. C* **119**, 1136-1145 (2015).♦
51. Y. He, J. Huang, B. G. Sumpter, A. A. Kornyshev, R. Qiao*, "Dynamic Charge Storage in Ionic Liquids-Filled Nanopores: Insight from a Computational Cyclic Voltammetry Study," *J. Phys. Chem. Lett.* **6**, 22-30 (2015).
52. Y. Liu, J. Huang, B. Yang, B. G. Sumpter, R. Qiao*, "Duality of the Interfacial Thermal Conductance in Graphene-Based Nanocomposites," *Carbon* **75**, 169-177 (2014).
53. X. Jiang, J, Huang, H. Zhao, B. G. Sumpter, R. Qiao*, "Dynamics of Electrical Double Layer Formation in Room-Temperature Ionic Liquids under Constant-Current Charging Conditions," *J. Phys.: Cond. Matter* **26**, 284109 (2014).
54. J. Zhou*, J. Huang, B. G. Sumpter, P. R. C. Kent, Y. Xie, H. Terrones, S. C. Smith, "Theoretical Predictions of Freestanding Honeycomb Sheets of Cadmium Chalcogenides," *J. Phys. Chem. C* **118**, 16236-16245 (2014).▽

55. J. Chen*, M. Shao, K. Xiao, A. J. Rondinone, Y.-L. Loo, J. E. Anthony, P. R. C. Kent, B. G. Sumpter, J. Huang, "Solvent-Type-Dependent Polymorphism and Charge Transport in a Long Fused-Ring Organic Semiconductor," *Nanoscale* **6**, 449-456 (2014).♦†
56. J. Zhou*, J. Huang, B. G. Sumpter, P. R. C. Kent, H. Terrones, S. C. Smith, Correction to "Structures, Energetics, and Electronic Properties of Layered Materials and Nanotubes of Cadmium Chalcogenides," *J. Phys. Chem. C* **117**, 26858-26858 (2013).
57. J. Zhou*, J. Huang, B. G. Sumpter, P. R. C. Kent, H. Terrones, S. C. Smith, "Structures, Energetics, and Electronic Properties of Layered Materials and Nanotubes of Cadmium Chalcogenides," *J. Phys. Chem. C* **117**, 25817-25825 (2013).†
58. D. Uhrig, G. C. Morar, M. Goswami, J. Huang, B. G. Sumpter, J. Zhou, S. M. Kilbey II, D. L. Pickel*, "Molecular Heterogeneity of Polystyrene-modified Fullerene Core Stars," *Macromolecules* **46**, 7451-7457 (2013).
59. X. Jiang, J. Huang, B. G. Sumpter, R. Qiao*, "Electro-Induced Dewetting and Concomittant Ionic Current Avalanche in Nanopores," *J. Phys. Chem. Lett.* **4**, 3120-3126 (2013).†
60. A. Lopez-Bezanilla*, J. Huang, P. R. C. Kent, B. G. Sumpter, "Tuning from Half-Metallic to Semiconducting Behavior in SiC Nanoribbons," *J. Phys. Chem. C* **117**, 15447-15455 (2013).
61. A. Lopez-Bezanilla*, J. Huang, H. Terrones, B. G. Sumpter, "Structure and Electronic Properties of Edge-Functionalized Armchair Boron Nitride Nanoribbons," *J. Phys. Chem. C* **116**, 15675-15681 (2012).
62. P. Wu, J. Huang, V. Meunier, B. G. Sumpter, R. Qiao*, "Voltage Dependent Charge Storage Modes and Capacity in Subnanometer Pores," *J. Phys. Chem. Lett.* **3**, 1732-1737 (2012).
63. P. Wu, J. Huang, V. Meunier, B. G. Sumpter, R. Qiao*, "Complex Capacitance Scaling in Ionic Liquid-Filled Nanopores," *ACS Nano* **5**, 9044-9051 (2011).
64. A. Lopez-Bezanilla*, J. Huang, H. Terrones, B. G. Sumpter, "Correction to Boron Nitride Nanoribbons Become Metallic," *Nano Lett.* **11**, 3879-3879 (2011).
65. A. Lopez-Bezanilla*, J. Huang, H. Terrones, B. G. Sumpter, "Boron Nitride Nanoribbons Become Metallic," *Nano Lett.* **11**, 3267-3273 (2011).†
66. J. J. Yoo, K. Balakrishnan, J. Huang, V. Meunier*, B. G. Sumpter, A. Srivastava, M. Conway, A. L. M. Reddy, J. Yu, R. Vajtai, P. Ajayan*, "Ultrathin Planar Graphene Supercapacitors," *Nano Lett.* **11**, 1423-1427 (2011).†
67. G. Feng, J. Huang, B. G. Sumpter, V. Meunier, R. Qiao*, "A "Counter-Charge Layer in Generalized Solvents" Framework for Electrical Double Layers in Neat and Hybrid Ionic Liquid Electrolytes," *Phys. Chem. Chem. Phys.* **13**, 14723-14734 (2011).
68. G. Feng, R. Qiao*, J. Huang, S. Dai, B. G. Sumpter, V. Meunier, "The Importance of Ion Size and Electrode Curvature on Electrical Double Layers in Ionic Liquids," *Phys. Chem. Chem. Phys.* **13**, 1152-1161 (2011).
69. J. Huang, B. G. Sumpter*, V. Meunier, Y. Tian, M. Kertesz*, "Cyclo-Biphenalenyl Biradicaloid Molecular Materials: Conformation, Tautomerization, Magnetism, and Thermochromism," *Chem. Mater.* **23**, 874-885 (2011).♦
70. G. Feng, R. Qiao*, J. Huang, B. G. Sumpter, V. Meunier, "Atomistic Insight on the Charging Energetics in Subnanometer Pore Supercapacitors," *J. Phys. Chem. C* **114**, 18012-18016 (2010).
71. J. Huang, R. Qiao, B. G. Sumpter, V. Meunier*, "Effect of Diffuse Layer and Pore Shapes in Mesoporous Carbon Supercapacitors," *J. Mater. Res.* **25**, 1469-1475 (2010).♦▽
72. J. Huang*, B. G. Sumpter, V. Meunier, G. Yushin, C. Portet, Y. Gogotsi*, "Curvature Effects in Carbon Nanomaterials: Exohedral versus Endohedral Supercapacitors," *J. Mater. Res.* **25**, 1525-1531 (2010).♦
73. C. Cagle, G. Feng, R. Qiao*, J. Huang, B. G. Sumpter, V. Meunier, "Structure and Charging Kinetics of Electrical Double Layers at Large Electrode Voltages," *Microfluid. Nanofluid.* **8**, 703-708 (2010).
74. G. Feng, R. Qiao*, J. Huang, B. G. Sumpter, V. Meunier*, "Ion Distribution in Electrified Micropores and its Role in the Anomalous Enhancement of Capacitance," *ACS Nano* **4**, 2382-2390 (2010).†
75. Y. Tian, J. Huang, M. Kertesz*, "Fluxional σ-bonds of 2,5,8-Tri-tert-butyl-1,3-diazaphenalenyl Dimers: Stepwise [3,3], [5,5] and [7,7] Sigmatropic Rearrangements via π-dimer Intermediates," *Phys. Chem. Chem. Phys.* **12**, 5084-5093 (2010).

76. G. Feng, J. Huang, B. G. Sumpter, V. Meunier, R. Qiao*, "Structure and Dynamics of Electrical Double Layers in Organic Electrolytes," *Phys. Chem. Chem. Phys.* **12**, 5468-5479 (2010).
77. Y. Li, A. J. Lampkins, M. B. Baker, B. G. Sumpter, J. Huang, K. A. Abboud, R. K. Castellano*, "Benzotrifuranone: Synthesis, Structure, and Access to Planar Heteroaromatics," *Org. Lett.* **11**, 4314-4317 (2009).
78. B. G. Sumpter*, J. Huang, V. Meunier, J. M. Romo-Herrera, E. Cruz-Silva, H. Terrones, M. Terrones, "A Theoretical and Experimental Study on Manipulating the Structure and Properties of Carbon Nanotubes Using Substitutional Dopants," *Int. J. Quant. Chem.* **109**, 97-118 (2009).
79. J. Huang*, B. G. Sumpter, V. Meunier, "A Universal Model for Nanoporous Carbon Supercapacitors Applicable to Diverse Pore Regimes, Carbon Materials, and Electrolytes," *Chem. Eur. J.* **14**, 6614-6626 (2008).♦Δ
80. J. Huang*, B. G. Sumpter, V. Meunier, "Theoretical Model for Nanoporous Carbon Supercapacitors," *Angew. Chem. Int. Ed.* **47**, 520-524 (2008).♦†‡ [ORNL press release at https://www.ornl.gov/news/packing-ions.]
81. J. Huang*, S. Kingsbury, M. Kertesz*, "Crystal Packing of TCNQ Anion π-Radicals Governed by Intermolecular Covalent π–π Bonding: DFT Calculations and Statistical Analysis of Crystal Structures, *Phys. Chem. Chem. Phys.* **10**, 2625-2635 (2008)."♦ [Invited contribution and dedicated to Prof. Roald Hoffmann on the occasion of his 70th birthday.]
82. J. Huang*, M. Kertesz*, "Theoretical Analysis of Intermolecular Covalent π–π Bonding and Magnetic Properties of Phenalenyl and Spiro-Biphenalenyl Radical π-Dimers," *J. Phys. Chem. A* **111**, 6304-6315 (2007).♦
83. J. Huang*, M. Kertesz*, "Intermolecular Covalent π–π Bonding Interaction Indicated by Bond Distances, Energy Bands, and Magnetism in Biphenalenyl Biradicaloid Molecular Crystal," *J. Am. Chem. Soc.* **129**, 1634-1643 (2007).♦
84. J. Huang, M. Kertesz*, "Stepwise Cope Rearrangement of Cyclo-Biphenalenyl via an Unusual Multicenter Covalent π-Bonded Intermediate," *J. Am. Chem. Soc.* **128**, 7277-7286 (2006).♦
85. J. Huang, M. Kertesz*, "One-Dimensional Metallic Conducting pathway of Cyclohexyl-Substituted Spiro-Biphenalenyl Neutral Radical Molecular Crystal," *J. Am. Chem. Soc.* **128**, 1418-1419 (2006).♦
86. J. Huang, M. Kertesz*, "Electronic Structures and Charge Transport Properties of the Organic Semiconductor Bis[1,2,5]thiadiazolo-*p*-quinobis(1,3-dithiole), BTQBT, and its Derivatives," *J. Phys. Chem. B* **109**, 12891-12898 (2005).♦
87. J. Huang, M. Kertesz*, "Validation of Intermolecular Transfer Integral and Bandwidth Calculations for Organic Molecular Materials," *J. Chem. Phys.* **122**, Article Number 234707 (2005).♦
88. J. Huang, M. Kertesz*, "Intermolecular Transfer Integrals for Organic Molecular Materials: Can Basis Set Convergence be Achieved?" *Chem. Phys. Lett.* **390**, 110-115 (2004).♦
89. J. Huang, M. Kertesz*, "Spin Crossover of Spiro-Biphenalenyl Neutral Radical Molecular Conductors," *J. Am. Chem. Soc.* **125**, 13334-13335 (2003).♦
90. J. Huang*, X. Sun, Z. Chen, Z. Li, "Research Overview and Developing Trend of Purification Catalysts for Automotive Exhaust," *Sichuan Huagong Yu Fushi Kongzhi* (*Sichuan Chemical Industry and Corrosion Control*) **1**, 32-35 (1998) (in Chinese).♦
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).♦
92. Z. Zhou*, J. Huang, W. Hu, F. Yao, Y. Zhang, "Hydrogen Diffusion Studies of Microcrystalline and Crystalline $LaNi_{3.94}Si_{0.54}$ Films," *J. Alloys Compd.* **231**, 297-301 (1995).
93. J. Huang*, Z. Zhou, W. Hu, F. Yao, D. Song, "Short Communication – Hydrogen Diffusion Studies of Microcrystalline $LaNi_{3.94}Si_{0.54}$ Films Using the Electrochemical Permeation Technique," *Int. J. Hydrogen Energy* **20**, 849-851 (1995).♦
94. J. Huang*, Z. Zhou, F. Yao, Y. Zhang, "Diffusion of Hydrogen in Hydrogen Storage Alloys," *Gaojishu Tongxun* (*Chinese High Technology Letters*), **4**, 34-37 (1994) (in Chinese).♦
95. J. Huang*, Z. Zhou, F. Yao, G. Yang, "Diffusion of Hydrogen in Metals and Alloys," *Dianchi* (*Battery Bimonthly*), **24**, 69-73 (1994) (in Chinese).♦

96. X. Feng*, R. Chen, J. Huang, Z. Zhang, "Synthesis of 2-Aroylamino-5-Benzyl-1,3,4-Thiadiazoles and Studies on their Reactions with Benzaldehyde," *Gaodeng Xuexiao Huaxue Xuebao* (*Chemical Journal of Chinese Universities*), **14**, 65-67 (1993) (in Chinese).

Book Chapters

97. J. Zhou, H. Terrones, S. C. Smith, B. G. Sumpter, J. Huang*, "Two-Dimensional Layered Materials of ZnX and CdX (X = S, Se, Te)," in "Beyond Graphene, New Layered Nanomaterials: Theory, Experiment and Applications", Editors: Mauricio Terrones, Florentino Lopez-Urias, Humberto Terrones; Wiley-VCH, 2016, accepted – Invited contribution.♦
98. J. Huang*, R. Qiao, G. Feng, V. Meunier, B. G. Sumpter, "Modern Theories of Carbon-Based Electrochemical Capacitors," in "Supercapacitors: Materials, Systems, and Applications," Editors: François Béguin and Elzbieta Frackowiak; Wiley-VCH: 2013 – Invited contribution.♦
99. J. Huang, J. Jakowski, A. Beste, J. Younker, A. Vazquez-Mayagoitia, E. Cruz-Silva, M. Fuentes-Cabrera, A. Lopez-Bezanilla, V. Meunier, B. G. Sumpter*, "Advancing Understanding and Design of Functional Materials through Theoretical and Computational Chemical Physics," in "Practical Aspects of Computational Chemistry II: An Overview of The Last Two Decades and Current Trends," Editors: Jerzy Leszczynski, Manoj. K. Shukla, Helene de Rode; Springer: 2012 – Invited contribution.♦
100. J. Huang*, B. G. Sumpter, V. Meunier, "A Universal Model for Nanoporous Carbon Supercapacitors," in "Mesoporous materials," Editor: Lynn T. Burness; Nova Science: 2009 – Invited contribution.♦

Conference Proceedings

101. 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).
102. 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).
103. 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).
104. 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).
105. 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. Review of Group Research on Energy Conversion and Storage in the Past 15 years - supercapacitor, Li/S battery, electrochemical nitrogen fixation, hydrogen evolution, and oxygen reduction, The Seventh Edition of Global Energy Meet (GEM-2023), invited by Conference Organizer, Mar 06-08 (2023).
2. 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).
3. 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).
4. Graphene Nanoribbons (GNR): Understanding Reaction Mechanism, Briefing to Office of Naval Research Program Manager, CNMS, Oak Ridge, TN, invited by An-Ping Li, March 25 (2019).
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).

Funded Proposals (selected recent)

1. FY23 US DOE, EPSCoR Partnership for Theory-Guided Innovation of High-Performance Electrocatalysts for Carbon Dioxide Reduction, DOE EPSCoR awarded to Prof. Zhongfang Chen at University of Puerto Rico, Rio Piedras; approved budget $750,000.
2. FY22 ORNL LDRD, co-I for A Novel Membrane Contactor Based CO_2 Separation; approved budget for FY22 is $495,000.
3. FY22 ORNL LDRD, co-I for Electrochemical Non-aqueous CO_2 Reduction with Electron-Proton Mediators; approved budget for FY22 is $514,500.
4. FY22 ORNL LDRD, co-I for Synergetic Plasma - Electrocatalytic Conversion of CO_2 and N_2 to Urea; approved budge for FY22 is $230,000.
5. FY21 ORNL SEED, PI for Synergetic Effects of Ultrastrong Electric Field on CO_2 Electroreduction, merged with two other teams eventually when the project was funded and served as co-I for Dynamics of Carbon Dioxide Reactive Reduction under Extreme Environment; approved budget $150,000.

Graduate and Postdoctoral Advisors

Prof. Miklos Kertesz (Georgetown University)
Dr. Vincent Meunier and Dr. Bobby G. Sumpter (ORNL)

Postdoctoral Scholar Advised

Dr. Jia Zhou (then faculty at Harbin Institute of Technology)

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)

High School Students Advised

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