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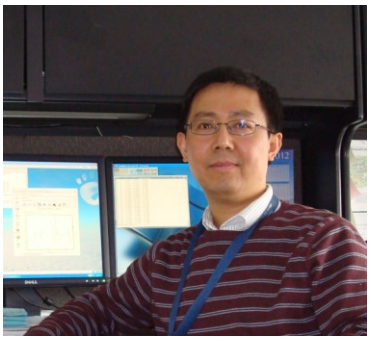
Publications



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

2010–p	Staff Scientist, ORNL
2007–2010	Postdoctoral Research Associate, ORAU/ORNL
2006–2007	Research Fellow, Chemistry Department, Georgetown University
1994–1999	Engineer, Southwest R&D Institute of Chemical Industry, Chengdu, China
2006–p	Reviewer for proposals of NSF, ACS PRF, ORNL, and various journals of American Chemical Society (ACS), American Physical Society (APS), Chinese Academy of Sciences (CAS), Elsevier, Institute of Physics (IOP), Multidisciplinary Digital Publishing Institute (MDPI), Royal Society of Chemistry (RSC), Springer, Wiley-VCH, and World Scientific

Honors and Awards

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

I received my bachelor's degree in Chemistry in 1991 and master's degree in 1994 in Physical Chemistry. My initial background was experimental Organic Chemistry and Physical Chemistry. Since 1999 I started to do computational and theoretical studies of material, physical, and chemical problems. I earned my Ph D in Physical Chemistry in 2006. Research interests are mainly the theoretical studies of electronic, optical, and magnetic properties of solid-state and low-dimensional materials, chemical reaction mechanism, and electrical energy conversion/storage. With a background of an experimental chemist and the expertise of a computational and theoretical chemist, my primary goal is to establish the bridge between experimental observations and theoretical rationalizations, which will hopefully lend supports for experimental materials optimizations.

Research Areas/Topics

1. *Structure-property correlations of organic and hybrid materials* through the modeling/theories of electronic structures of 0D through 3D materials including organic conjugated polymers, molecular materials of pentacene derivatives, anthradithiophene derivatives, BTQBT, and hybrid $CH_3NH_3PbI_3$. In addition to organic and hybrid materials, we are also interested in *layered and/or nanostructured inorganic materials* such as graphene, SiC, BN, and Cd (or Zn) chalcogenides of the 0D, 1D, and 2D. These materials are important for applications in electronic devices such as light-emitting diodes, photovoltaics, field effect transistors, magnetooptics, spintropics, etc. The

calculations of electronic properties include crystal orbitals, band structures, density of states, 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, and ionization potential. We employ tight binding model, DFT, time-dependent DFT, quasiparticle GW approximation, and Bethe Salpeter Equation (BSE) to understand the electronic, optical, and magnetic properties. We are interested in charge and spin density wave phenomena.

2. *Unusual multicenter covalent pi-pi bonding interactions* of long distance (~3Å) between organic pi-radicals or biradicaloids. Typical examples are phenalenyl and spiro-biphenalenyl derivatives, and TTF-TCNQ which are exploited as the building blocks. 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 pi-pi stacking and the magnetic exchanges between neighboring unpaired spins are deeply rooted in the novel multicenter covalent pi-pi bondings. Since chemical bonds usually go hand in hand with magnetism, we study the weak pi-pi 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 optical, electric, or magnetic properties due to the change of external stimuli, and thus making these materials "smart".
3. *Electrical energy conversion/storage* with supercapacitors, Li-S batteries, and solid-state proton exchange electrolytes. 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 and are also testing these materials for Li^+ conduction.

Peer Reviewed Journal Publications

1. G. Hu, V. Fung, J. Huang, P. Ganesh, "Work Function Engineering of 2D Materials: The role of Polar Edge Reconstructions," *Nano Lett.* submitted (2020).
2. 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 Ti3C2 MXene Films across Length Scales," *Energy Environ. Sci.* **13**, 2549-2558 (2020).
3. 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).
4. 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).
5. 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).
6. 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).
7. 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).

8. 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).
9. 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).
10. 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).
11. 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).
12. 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).
13. A. J. Rondinone, J. Huang, "Geometry Aids Green Carbon Electrochemistry," *Nat. Catal.* **1**, 903-904 (2018).
14. 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(-caprolactone)s: Synthesis and Isotope Effects on the Crystal Structures and Properties," *Macromolecules* **51**, 9393-9404 (2018).
15. 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).
16. 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).
17. 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).
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21. 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).
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23. 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).
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Small Molecule Organic Semiconductor Thin Films Fabricated by Slow Solution Crystallization," *Nanoscale* **6**, 449-456 (2014).

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