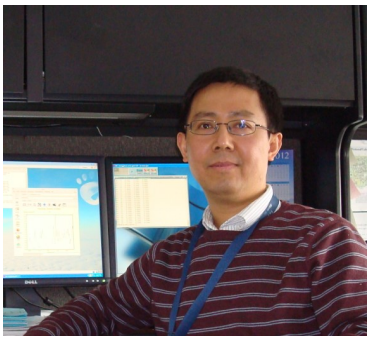
# Jingsong Huang

R&D Staff
Nanomaterials Theory Institute
Center for Nanophase Materials Sciences (CNMS)
Computational Chemical and Materials Sciences Group
Computional Sciences & Engineering Division (CSMD)
Oak Ridge National Laboratory
(865) 576-3991
huangj3@ornl.gov
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 | Postdoc, CSMD, 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 and ORNL and various journals of American Chemical Society, American Physical Society, Chinese Academy of Sciences, Elsevier, Institute of Physics, Royal Society of Chemistry, Springer, Wiley-VCH, and World Scientific |

**Honors and Awards**

| | |
|---|---|
| 2015 | Distinguished Award for a Scientific or Technical Contribution, CSMD, ORNL |
| 2012 | Distinguished Scientific Paper Published, CSMD, ORNL |
| 2008 | IBM-Löwdin Fellowship, the 48$^{th}$ 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 from Southwest China Normal University (currently known as Southwest University) in 1991 and master's degree in 1994 in Physical Chemistry from Nankai University. Prior to study abroad, I worked as an engineer at the Southwest Research & Design Institute of Chemical Industry. My initial background was experimental Organic Chemistry and Physical Chemistry. Since 1999 I decided to pursue theoretical research using computational chemistry. I earned my Ph D in Physical Chemistry in 2006 from Georgetown University. Research interests are mainly the theoretical studies of the electronic, optical, and magnetic properties of solid-state and low-dimensional materials, chemical reaction mechanism, and electrical energy 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, and 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 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 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. K. Tu, F. Li, J. Gu, Y. Tian, B. G. Sumpter, J. Huang, Z. Chen, "Pancake Bond Formation in Graphene Bilayers Enabled by B Doping, N Doping, and B/N Co-Doping," in preparation (2018).
2. Z. Yu, J. Huang, B. G. Sumpter, R. Qiao, "Electrified Interfaces of Solvate Ionic Liquids" in preparation (2018).
3. 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," in revision (2018).
4. J. Jakowski, J. Huang, B. G. Sumpter, S. Garashchuk, "Theoretical Assessment of the Nuclear Quantum Effects on Polymer Crystallinity via Perturbation Theory and Dynamic," under review (2018).
5. 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," under review (2018).
6. 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).
7. 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).
8. 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).

9. 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).
10. 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).
11. Z. Yu, F. Zhang, J. Huang, B. G. Sumpter, R. Qiao, "Ionic Liquids-Mediated Interactions between Nanorods*," J. Chem. Phys.* **147**, 134704 (2017).
12. 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).
13. 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, "Ionic Migration in Grain Boundaries of Organometallic Halide Perovskite Films: Suppressed by Fullerene and Enhanced by Chlorine," *Adv. Funct. Mater.* **27**, 1700749 (2017).
14. W. Cui, S. Xu, B. Yan, Q. Xu, B. G. Sumpter, J. Huang, S. Yin, H.-J. Zhao, Y. Wang, "Triphasic Two-Dimensional Materials by Vertically Stacking Laterally Heterostructured 2H-/1T-$MoS_2$ on Graphene for Enhanced Photoresponse," *Adv. Electron. Mater.* **3**, 1700024 (2017).
15. F. Zhang, Y. He, J. Huang, B. G. Sumpter, R. Qiao, "Multi-Component Gas Storage in Organic Cage Molecules," *J. Phys. Chem.* **121**, 12426-12433, (2017).
16. C. Hu, X. Zeng, Y. Liu, M. Zhou, H. Zhao, T. M. Tritt, J. He, J. Jakowski, P. R. C. Kent, B. G. Sumpter, J. Huang, "Density Functional Theory Studies of Partial La Filling and Sb Vacancy Defects in $CoSb_3$ Skutterudites," *Phys. Rev. B* **95**, 155204 (2017).
17. 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).
18. J. Lee, J. Huang, B. G. Sumpter, M. Yoon, "Strain-Engineered Optoelectronic Properties of Two-Dimensional Transition Metal Dichalcogenide Lateral Heterostructures," *2D Mater.* **4**, 021016 (2017).
19. 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," *Nanotech.* **27**, 424002 (2016).
20. 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).
21. 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).
22. 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).
23. 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).
24. Y. Tian, B. G. Sumpter, S. Du, J. Huang, "Pancake Pi-Pi Bonding Goes Double: Unexpected 4e/All-Sites Bonding in Boron- and Nitrogen-Doped Phenalenyls," *J. Phys. Chem. Lett.* **6**, 2318-2325 (2015).
25. 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).
26. 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).
27. 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).
28. 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).

29. 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).
30. 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).
31. 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). Journal cover highlight.
32. 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 Crystalline Polymorphism of High Performance, Small Molecule Organic Semiconductor Thin Films Fabricated by Slow Solution Crystallization," *Nanoscale* **6**, 449-456 (2014).
33. J. Zhou, J. Huang, B. G. Sumpter, P. R. C. Kent, H. Terrones, S. C. Smith, "Structures, Energetics, and Electronic Properties of Cadmium Chalcogenides," *J. Phys. Chem. C* **117**, 25817-25825 (2013).
34. 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).
35. 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).
36. 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).
37. 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).
38. 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).
39. 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).
40. A. Lopez-Bezanilla, J. Huang, H. Terrones, B. G. Sumpter, "Boron Nitride Nanoribbons Become Metallic," *Nano Lett.* **11**, 3267-3273 (2011).
41. 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). Thomson Reuters Highly Cited Article.
42. 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).
43. 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).
44. 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).
45. 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).
46. 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). Journal cover highlight.
47. 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).
48. 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).

49. 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).
50. Y. Tian, J. Huang, M. Kertesz, "Fluxional Sigma-bonds of 2,5,8-Tri-tert-butyl-1,3-diazaphenalenyl Dimers: Stepwise [3,3], [5,5] and [7,7] Sigmatropic Rearrangements via Pi-dimer Intermediates," *Phys. Chem. Chem. Phys.* **12**, 5084-5093 (2010).
51. 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).
52. 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).
53. 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).
54. 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). Thomson Reuters Highly Cited Article.
55. J. Huang, B. G. Sumpter, V. Meunier, "Theoretical Model for Nanoporous Carbon Supercapacitors," *Angew. Chem. Int. Ed.* **47**, 520-524 (2008). Thomson Reuters Highly Cited Article.
56. J. Huang, S. Kingsbury, M. Kertesz, "Crystal Packing of TCNQ Anion Pi-Radicals Governed by Intermolecular Covalent Pi-Pi 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.
57. J. Huang, M. Kertesz, "Theoretical Analysis of Intermolecular Covalent Pi-Pi Bonding and Magnetic Properties of Phenalenyl and Spiro-Biphenalenyl Radical Pi-Dimers," *J. Phys. Chem. A* **111**, 6304-6315 (2007).
58. J. Huang, M. Kertesz, "Intermolecular Covalent Pi-Pi Bonding Interaction Indicated by Bond Distances, Energy Bands, and Magnetism in Biphenalenyl Biradicaloid Molecular Crystal," *J. Am. Chem. Soc.* **129**, 1634-1643 (2007).
59. J. Huang, M. Kertesz, "Stepwise Cope Rearrangement of Cyclo-Biphenalenyl via an Unusual Multicenter Covalent Pi-Bonded Intermediate," *J. Am. Chem. Soc.* **128**, 7277-7286 (2006).
60. 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).
61. 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).
62. J. Huang, M. Kertesz, "Validation of Intermolecular Transfer Integral and Bandwidth Calculations for Organic Molecular Materials," *J. Chem. Phys.* **122**, Article Number 234707 (2005).
63. J. Huang, M. Kertesz, "Intermolecular Transfer Integrals for Organic Molecular Materials: Can Basis Set Convergence be Achieved?" *Chem. Phys. Lett.* **390**, 110-115 (2004).
64. J. Huang, M. Kertesz, "Spin Crossover of Spiro-Biphenalenyl Neutral Radical Molecular Conductors," *J. Am. Chem. Soc.* **125**, 13334-13335 (2003).
65. 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).
66. 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).
67. 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).
68. 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).

69. 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).
70. J. Huang, Z. Zhou, F. Yao, G. Yang, "Diffusion of Hydrogen in Metals and Alloys," *Dianchi* (*Battery Bimonthly*), **24**, 69-73 (1994) (in Chinese).
71. 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**

72. Jia Zhou, Humberto Terrones, Sean C. Smith, Bobby G. Sumpter, Jingsong Huang, "Two-Dimensional Layered Materials of ZnX and CdX (X = S, Se, Te)," in "Beyond Graphene, New Layered Nanomaterials: Theory, Experiment and Applications", Editors: Mauricio Terrones, Florentino Lopez-Urias, Humberto Terrones; Wiley-VCH, 2016 – Invited contribution.
73. 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.
74. 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.
75. 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**

76. 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).
77. 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).
78. G. Feng, R. Qiao, J. Huang, B. G. Sumpter, V. Meunier, "Computational Modeling of Carbon Nanostructures for Energy Storage Applications," Proceeding of the 2010 10$^{th}$ IEEE Conference on Nanotechnology, NANO 2010, Article number 5698075, pp 100-104 (2010).
79. 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**

1. Computational Modeling of Carbon-Based Supercapacitors, 47$^{th}$ Central Regional Meeting of ACS, Covington, KY, May 18-21 (2016).
2. Capacitive Energy Storage Using Carbon Supercapacitors: from Modeling to Device, Nanostructured Materials for Lithium Ion Batteries and for Supercapacitors, 2013 TMS Annual Meeting & Exhibition, San Antonio, TX, March (2013).
3. Modeling Capacitive Energy Storage in Carbon Nanosystems, Theory and Simulation of Nano Scale Materials, CINT, Sandia National Laboratory, Albuquerque, New Mexico, October (2010).
4. Capacitor models for various regimes, carbons, and electrolytes, The 9$^{th}$ International Advanced Automotive Battery & EC Capacitor Conference, Long Beach, CA, June (2009).

**Workshop/Conference Organization and Session Chair**

1. Panel discussion, The 9$^{th}$ Advanced Automotive Battery & EC Capacitor Conference (AABC-09), Long Beach, CA, June (2009).

2. Session chair, The International Conference on Theory and Application of Computational Chemistry, Shanghai, China, September (2008).

**Collaborations over Last 5 Years**
Prof. John E. Anthony, University of Kentucky; Dr. Shih-Hung Chou, 3M Company; Prof. Pravas Deria, Southern Illinois University-Carbondale; Prof. Jian He, Clemson University; Prof. Miklos Kertsz, Georgetown University; Prof. Zhi-Ru Li, Jili University, China; Prof. Vincent Meunier, Rensselaer Polytechnic Institute; Dr. Adam Miller, 3M Company; Prof. Humberto Terrones, Rensselaer Polytechnic Institute; Prof. Yong-Hui Tian, Sichuan University, China; Prof. Terry M. Tritt, Clemson University; Prof. Rui Qiao, Virginia Tech; Dr. Yun Wang, Griffith University, Australia; Prof. Hui Zhao, University of Nevada

**Graduate and Postdoctoral Advisors**
Prof. Miklos Kertesz (Georgetown University), Dr. Vincent Meunier and Dr. Bobby G. Sumpter (ORNL)

**Postdoctoral Scholar Mentored**
Dr. Jia Zhou (then faculty at Harbin Institute of Technology)

**Graduate Students Mentored**
Lili Qiu (Georgetown University)
Chongze Hu (University of Minnesota Twin Cities)

**High School Student Mentored**
Peter Ni (Montgometry High School, Skillman, NJ)