

Zhiyong Zhang

Software Developer, Research, Research Computing Op Budget

Bio

CURRENT ROLE AT STANFORD

High Performance Computing Research

HONORS AND AWARDS

- Science and Technology Award, 1st Prize, Shaanxi Province (China) (1998)
- University graduate fellowship, Ohio State University (1998)
- Fellowship, Associated Western Universities (2001 to 2004)

EDUCATION AND CERTIFICATIONS

- BS, Hebei University , Physics (1985)
- MS, Northwestern University , Computational Chemistry (1988)
- Bioinformatics Certificate, Stanford University , Bioinformatics (2003)
- MS, Ohio State University , Computer Science and Information System (1998)
- PHD, Ohio State University , Chemical Physics (1998)

Publications

PUBLICATIONS

- **Theoretical study of CDW phases for bulk NbX₂ (X = S and Se).** *Physical chemistry chemical physics : PCCP*
Du, H., Jiang, Z., Zheng, J., Zhang, X., Wang, W., Zhang, Z.
2024
- **Design Principles for Rotational Cluster Anion [BH₄]⁽⁻⁾ Promote Superionic Conductivity in Sodium-Rich Antiperovskite Na₃OBH₄** *JOURNAL OF PHYSICAL CHEMISTRY C*
Zhao, Q., Guo, J., Su, M., Suo, B., Zhu, H., Zhou, B., Zhang, Z., Song, Q.
2022
- **Theoretical study of the synthesis, characterization and hydrogen storage properties of a high-density hydrogen storage material: (CH₃NH₃)BH₄** *INTERNATIONAL JOURNAL OF HYDROGEN ENERGY*
Zhao, Q., Chen, L., Suo, B., Zhang, Z., Deng, D., Zhou, B., Zhu, H., Song, Q.
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- **--Peroxo Species Formed in the Bulk of Silicate Cathodes.** *Angewandte Chemie (International ed. in English)*
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2021
- **Tuning conduction mechanism via surface termination and point defects in n-type LaAlO₃/SrTiO₃ interfaces**
Guan, L., Tan, F., Liang, Y., Xu, X., Han, S., Guo, J., Wang, J., Zhang, Z., Li, X.
ELSEVIER.2021
- **The mechanism of V-modification in Li₂CoSiO₄ cathode material for Li-ion batteries: A combined first-principles and experimental study** *ELECTROCHIMICA ACTA*

- Huai, L., Du, W., Zhang, Z., Zhang, X., Zhang, Z., Chen, Z., Wu, J., Wang, D., Li, J.
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- **Theoretical study on martensitic-type transformation path from rutile phase to α -PbO(2) phase of Ti₂(O)*** *CHINESE PHYSICS B*
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 - **NWChem: Past, present, and future.** *The Journal of chemical physics*
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 - **The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry.** *The Journal of chemical physics*
Lischka, H., Shepard, R., Muller, T., Szalay, P. G., Pitzer, R. M., Aquino, A. J., Araujo do Nascimento, M. M., Barbatti, M., Belcher, L. T., Blaudeau, J., Borges, I. J., Brozell, S. R., Carter, et al
2020; 152 (13): 134110
 - **Origin of the structural diversity of the alkaline metal borohydride MBH₄ (M = Li, Na, K, Rb and Cs): Insights from first-principles calculations** *INTERNATIONAL JOURNAL OF HYDROGEN ENERGY*
Zhao, Q., Song, Q., Zhu, H., Zhang, Z., Jiang, Z., Zhou, B.
2020; 45 (16): 9946–58
 - **Effects of the Dopant Site on the Absorption Properties of CsPb_{1-x}M_xI₂Br (M = Ge, Sn, Sr, and Cu): A First-Principles Investigation** *JOURNAL OF PHYSICAL CHEMISTRY C*
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 - **Theoretical study on transport-scheme conversion of g-C₃N₄/TiO₂ heterojunctions by oxygen vacancies** *Applied Surface Science*
Yan, M.
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 - **A first-principles simulation of the metal borohydride ammonia borane complex (LiBH₄)(2)(NH₃BH₃) and the decomposition reaction pathway for hydrogen storage** *INTERNATIONAL JOURNAL OF HYDROGEN ENERGY*
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 - **Comparison of geometry models in the study of perovskite heterostructures** *APPLIED SURFACE SCIENCE*
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 - **Theoretical study of disorder-order transition of sodium borohydride** *COMPUTATIONAL MATERIALS SCIENCE*
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 - **Formation of charge-transfer complexes significantly improves the performance of polymer solar cells based on PBDTTT-C-T: PC71BM** *PROGRESS IN PHOTOVOLTAICS*
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 - **Formation of charge transfer complexes significantly improves the electron transfer process of polymer solar cells** *ORGANIC ELECTRONICS*
Fu, G., Wang, T., Cai, J., Shi, J., Luo, Z., Li, G., Li, X., Zhang, Z., Yang, S.
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 - **Complexation of Curium(III) with DTPA at 10-70 degrees C: Comparison with Eu(III)-DTPA in Thermodynamics, Luminescence, and Coordination Modes** *INORGANIC CHEMISTRY*
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- **Spin-orbit DFT with analytic gradients and applications to heavy element compounds** *THEORETICAL CHEMISTRY ACCOUNTS*
Zhang, Z.
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- **Correlation of intercalation potential with d-electron configurations for cathode compounds of lithium-ion batteries** *Phys. Chem. Chem. Phys*
Chen, Z., Zhang, C., Zhang, Z., Li, J.
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- **Formation of charge transfer complexes significantly improves the performance of polymer solar cells based on PBDTTT-C-T: PC71BM** *Prog. Photovolt: Res. Appl.*
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2014
- **Exotic Topological Insulator States and Topological Phase Transitions in Sb₂Se₃-Bi₂Se₃ Heterostructures** *ACS NANO*
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- **First principles investigation of electronic structure change and energy transfer by redox in inverse spinel cathodes LiNiVO₄ and LiCoVO₄** *JOURNAL OF MATERIALS CHEMISTRY*
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- **Electrochemical quantum tunneling for electronic detection and characterization of biological toxins** *Conference on Micro- and Nanotechnology Sensors, Systems, and Applications IV*
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- **Sequestering uranium from seawater: binding strength and modes of uranyl complexes with glutarimidedioxime** *DALTON TRANSACTIONS*
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- **Fermi Level Unpinning and Schottky Barrier Modification by Ti, Sc and V Incorporation at NiSi₂/Si Interface** *CHINESE PHYSICS LETTERS*
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- **The Role of Free N-Heterocyclic Carbene (NHC) in the Catalytic Dehydrogenation of Ammonia-Borane in the Nickel NHC System** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
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- **Configuration interaction studies on the electronic states of the CUO molecule** *MOLECULAR PHYSICS*
Yang, T., Tyagi, R., Zhang, Z., Pitzer, R. M.
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- **C-H bond formation at the graphite surface studied with core level spectroscopy** *SURFACE SCIENCE*
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2002
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- **NEW REALIZATION OF LOOP DRIVEN DIRECT CI** *JOURNAL OF COMPUTATIONAL CHEMISTRY*
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- **ALTERNATIVE IMPLEMENTATION OF THE UNITARY-GROUP APPROACH TO THE ATOMIC SHELL THEORY** *INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY*
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