Zisheng LI

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Education

University of Oxford — Oxford, UK
- DPhil in Inorganic Chemistry — Oct 2021 – present

Renmin University of China — Beijing, China
- Bachelor of Science in Chemistry (GPA: 3.8/4.0) — Sept 2017 – June 2021

Research Interests

My research focuses on the theoretical analysis of the electronic configurations of open-shell Zintl clusters, including multi-center metal-metal bonding, cluster growth mechanisms, magnetic properties, *etc.* with DFT. The related work establishes the connection between our clusters and existing closed-shell counterparts, contributing to the understanding of the metal-metal bonding and geometry distortions of the clusters based on Kohn-Sham orbitals. For strongly correlated clusters with direct interactions between transition metals, we revisit the electronic properties using advanced methods such as DMRG, CASSCF for static correlation, and CASPT2 or MCPDFT for dynamic correlation with a large active space. We aim to obtain a reliable ground state description and to scrutinize the metal-metal bonding in a spin-adapted manner.

Publications

6. **Fe–Fe bonding in the rhombic Fe_4 cores of the Zintl clusters $[Fe_4E_{18}]^{4-}$ (E = Sn and Pb)**
   W.-X. Chen‡, **Z.-S. Li**‡, H. W. T. Morgan, C.-C. Shu, Z.-M. Sun* and J. E. McGrady*
   Chem. Sci., 2024, **15**, 4981-4988.

5. **Snap-shots of cluster growth: structure and properties of a Zintl ion with an Fe_3 core, $[Fe_3Sn_{18}]^{4-}$**
   Z.-S. Li‡, W.-X. Chen‡, H. W. T. Morgan, C.-C. Shu, Z.-M. Sun* and J. E. McGrady*
   Chem. Sci., 2024, **15**, 1018-1026.

4. **Metal-metal bonds in Zintl clusters: Synthesis, structure and bonding in $[Fe_2Sn_4Bi_8]^{3-}$ and $[Cr_2Sb_{12}]^{3-}$**
   Y.-N. Yang‡, **Z.-S. Li**‡, S. Mondal, L. Qiao, C.-C. Wang, W.-J. Tian, Z.-M. Sun* and J. E. McGrady*.
   Chin. Chem. Lett., 2024, **35**, 109048 (Link to the corresponding poster presented in APATCC10)

3. **Synthesis and characterization of $[Fe_3(As_3)_3(As_4)]^{3-}$, a binary Fe/As Zintl cluster with an Fe_3 core**
   W.-Q. Zhang‡, **Z.-S. Li**‡, J. E. McGrady* and Z.-M. Sun*
   Angew. Chem. Int. Ed., 2023, **62**, e202217316.

Before PhD

2. **$Ln_3@C_{80}^+$ (Ln = lanthanide): a new class of stable metallofullerene cations with multicenter metal–metal bonding in the sub-nanometer confined space**
   Y. Jiang, **Z. Li**, Y. Wu and Z. Wang*
   Inorg. Chem. Front., 2022, *9*, 2173-2181.

1. **Activation of the unreactive bond in C_{70} fullerene toward Diels-Alder reaction by encapsulation of a lithium atom**
   Z. Li, Y. Jiang, Y. Wu and Z. Wang*
   Chem. Asian J., 2020, **15**, 3096-3103.

Teaching Experience

Demonstrator on Computational Chemistry — 2022-2024
- S112 - Introduction to Computational Chemistry
- S212 - Energy Profiles in Computational Chemistry
- S218 - Introductory Python for Chemists
- S219 - An Introduction to Coding in MATLAB

Computational Skills

Computational Chemistry Software:

- GM search: ABCluster
- DFT calculations: ADF, Gaussian, Orca
- Post-HF calculations: OpenMolcas (QCMaquis, Block 2.0), PySCF (Block 2.0)
- GUIs: ChemCraft, Avogadro, Multiwfn

Operating System: Linux (HPC), MacOS

Programming: Python, Shell scripts

Awards

1. **Class 2021 Outstanding Graduate of Renmin University of China**
2. **2023 Chinese Government Award for Outstanding Self-financed Students Abroad** by Chinese Scholarship Council (CSC)