Min-Ye Zhang

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Education

2015.9 – **College of Chemistry and Molecular Engineering, Peking University.**
Graduate student (2020 graduation), Theoretical and Computational Chemistry. Advisor: Prof. Hong Jiang

2011.9 – 2015.7 **College of Chemistry and Molecular Engineering, Peking University.**
B. Sc. in Chemistry. GPA: 3.41/4

Skills

Theory Tools	Density functional theory, many-body theory	Softwares	VASP, WIEN2K, ABINIT, GPAW, FHI-GAP
Programming	Python, Fortran, Shell/Bash, MPI, C (basics)	Libraries	Intel® MKL, spglib, FFTW3, PHONOPY, ASE
Dev. Tools	Vim, VS Code, Git, Makefile, Mathematica®	Visualization	Matplotlib, XmGrace, Adobe® Photoshop
Document	LaTeX, Markdown, Jupyter Notebook	Foreign Lang.	CET6 (550), JLPT N1 (113)

Experience

Scientific Projects

2017.9 – **Development and Implementation of First-principles Electronic Structure Method Beyond Density Functional Theory Within LAPW Framework**, *Ph.D. project*.
- Test, maintain and optimize the home-brew Fortran program FHI-GAP for all-electron *GW* calculations based on many-body perturbation theory.
- Derived the representation of truncated Coulomb interaction within mixed product basis, and demonstrated its efficient acceleration for the convergence of self-energy of low-dimensional electronic systems with respect to the vacuum size.
- Implemented all-electron ACFDT-RPA functionality, and tested its interface to WIEN2K and reliability of parallelization.

2016.8 – 2017.3 **Theoretical Study on the Catalytic Performance of Core-Shell Fe@FeP Nanoparticles for Hydrogen Generation Reaction (HER)**, *collaborative project*.
- Built atomistic models for Fe@FeP and their H-adsorption counterparts with different interfaces, surfaces and adsorption sites, and perform first-principles calculations for total energy.
- Demonstrated the exceptional catalytic performance observed experimentally by predicting a close-to-zero change in Gibbs free energy for the anode reaction at Fe@FeP, with calculations taking zero-point energy and vibration entropy into account.

2015.12 – 2018.4 **Theoretical Study on Thermodynamic Stability of Iron Disulfide FeS_2 Polymorphs**, *Ph.D. project*.
- Correctly reproduced the experimentally observed enthalpy of transformation from FeS_2 pyrite phase to marcasite by accurate ACFDT-RPA calculation and vibrational zero-point energy from phonon calculation.
- Interpreted the thermodynamic stability of pyrite by designing an effective bandgap as a descriptor of band structure to capture the trend of RPA correlation energy when varying crystal volume.

2017.10 – **Python Scripts Set `mykit` for Pre- and Post-Processing IOs of First-principles Code Packages**, *independent code*.
- Support several famous packages and use keyword mapping to allow conversion between input files for different packages.
- Open-sourced on GitHub. Continuous integration, automatic test and coverage (77.2% with 4061 SLOC).

Student Affairs

2015.9 – 2017.7 **Branch Secretary**, *CCP branch of graduate students from Class 2015, CCME, PKU.*

Publications

2019.9 – **1st author**, *Preprint*, Electronic Band Structure of Cuprous and Silver Halides: an All-Electron *GW* Study. arXiv:1906.02472 (2019).

2018.10 – **3rd author**, *IF=7.329*, Doubly Screened Hybrid Functional: an Accurate First-Principles Approach for Both Narrow- and Wide-Gap Semiconductors. *J. Phys. Chem. Lett.* **2018**, *9*, 2338-2345.

2018.3 – **1st author**, *IF=10.733*, Relative Stability of FeS_2 Polymorphs with the Random Phase Approximation Approach. *J. Mater. Chem. A* **2018**, *6*, 6606.

Awards

2017.10 – **Xianfeng Scholarship for Phys. Chem.**, *PKU*.

2016.10 – **President's Ph.D. Scholarship**, *PKU*.

2015 – 2019 **Merit Student** ×3, *PKU*.

2011 – 2015 **Wusi Scholarship, Xianfeng Scholarship**, *PKU*.

Miscellanies

- **Teaching Assistant**: Comprehensive Physical Chemistry (2017 and 2018 Spring semesters).
- **Translation**: Japanese interview and subtitle. General scientific article for publication in *Scientific American* (Chinese).
- **Blog**: technical writings on scientific programming and computation at homepage.
- **Sports**: running, basketball, softball