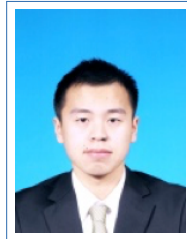


Min-Ye Zhang

No. 5 Yiheyuan Rd, Haidian Dist.
100871 Beijing
☎ +86 188 1050 7549
✉ stevezhang@pku.edu.cn
📧 shigaro.org
🌐 <https://github.com/minyez>



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 FeS₂ Polymorphs, *Ph.D. project.*

- Correctly reproduced the experimentally observed enthalpy of transformation from FeS₂ 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 FeS₂ 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

Merit Student ×3, PKU.

2019

Wusi Scholarship, Xianfeng Scholarship, PKU.

2011

2015

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