张旻烨

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教育背景

2015.9 **北京大学 化学与分子工程学院**, 博士研究生, 理论与计算化学 (预期 2020 年毕业). 导师：蒋鸿 研究员.

2011.9 – 2015.7 **北京大学 化学与分子工程学院**, 理学学士, 化学, GPA: 3.41/4.

技能

理论工具	密度泛函理论, 多体理论	**计算软件**	VASP, WIEN2K, ABINIT, GPAW, FHI-GAP
编程语言	Python, Fortran, Bash, MPI 并行, C (基础)	**科学库**	Intel® MKL, spglib, FFTW3, PHONOPY, ASE
开发工具	Vim, VS Code, Git, Makefile, Mathematica®	**可视化**	Matplotlib, XmGrace, Adobe® Photoshop
文档写作	LaTeX, Markdown, Jupyter Notebook	**外语能力**	CET6 (550), JLPT N1 (113)

经历

科研项目

2017.9 – **基于 LAPW 框架的超越密度泛函理论的第一性原理电子结构方法研究与程序开发**, 博士课题.
- 调试 / 维护 / 优化课题组自研的多体微扰理论 *GW* 全电子计算 Fortran 程序 FHI-GAP;
- 推导混合基组下的截断库仑势，实现低维材料体系自能关于模型参数的加速收敛;
- 实现 ACFDT-RPA 电子相关能全电子计算，调试与 WIEN2K 的接口，测试并行可靠性.

2016.8 – 2017.3 **核壳结构 Fe@FeP 纳米颗粒催化氢产生反应的理论研究**, 合作课题.
- 构建 Fe@FeP 界面表面模型与不同表面位点的氢吸附模型，进行密度泛函的第一性原理计算;
- 在考虑零点能与振动熵情况下验证了 Fe@FeP 阴极反应自由能变接近于零，佐证其实验上优良催化性能.

2015.12 – 2018.4 **二硫化亚铁FeS_2 晶相平衡态热稳定性的理论研究**, 博士课题.
- 基于 ACFDT-RPA 方法，在计算上首次得到与实验值处于同一数量级的FeS_2 黄铁矿相到白铁矿相的转化焓;
- 通过构造有效带隙描述符，从电子结构差别上解释了黄铁矿相热稳定性来源及传统密度泛函近似失效的原因.

2017.10 – **从头算程序输入输出文件前后处理的 Python 脚本集 `mykit`**, 独立项目.
- 适用于多种从头算程序，实现关键词映射，允许不同程序输入文件的近似相互转换;
- GitHub 开源. 支持连续集成、自动化测试与覆盖度计算 (4061 行 77.2%).

学生工作

2015.9 – 2017.7 **支部书记**, 北京大学化学与分子工程学院 *2015* 级研究生党支部.
- 统筹支部党员发展、策划党团日活动、定期召开支部生活会和党员大会;
- 组织党团日获校级三等奖 (2016)，本人获评学院优秀党员.

2011.9 – 2015.7 **班长**, 北京大学化学与分子工程学院 *2011* 级本科生一班.

论文发表

2019.9 – **第一作者**, 预印本, Electronic Band Structure of Cuprous and Silver Halides: an All-Electron *GW* Study. arXiv:1906.02472 (2019).

2018.10 – **第三作者**, *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 – **第一作者**, *IF=10.733*, Relative Stability of FeS_2 Polymorphs with the Random Phase Approximation Approach. *J. Mater. Chem. A* **2018**, *6*, 6606.

获得奖项

2017.10 – **先锋物理化学奖学金**, 校级.

2016.10 – **校长奖学金, 王世仪奖学金**, 校级.

2015 – 2019 **三好学生** (×3), **三好学生标兵**, 校级.

2011 – 2015 **五四奖学金, 先锋奖学金**, 校级.

其他活动

- **助教** 中级物理化学 (2017、2018 春季学期).
- **翻译** 日语访谈和字幕制作；英文科普文章，即将发表于《环球科学》杂志.
- **博客** 搭建个人主页撰写科学计算相关技术博客.
- **跑步** 舒缓压力. 7 公里配速 4’30.
- **篮球** 担任院队首发，蝉联北大硕博杯院系篮球赛冠军.

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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 – **Principal 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