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EDUCATION

My research interest is in prediction and design of functional materials with computational chemistry or machine learning techniques, focusing on covalent organic frameworks (COFs) and metal-organic frameworks (MOFs), especially their electronic structures, magnetic, catalytic and charge transport properties.

EDUCATION

04/2022-now	Humboldt Postdoctoral Fellow Technische Universität Dresden, Germany (Advisor: Prof. Thomas Heine)
05/2021-10/2021	Research Assistant Tsinghua University, P. R. China (Advisor: Prof. Zhigang Shuai)
08/2015-04/2021	Ph.D. in Physical Chemistry, Tsinghua University, P. R. China (Advisor: Prof. Dong Wang)
07/2014-09/2014	Visiting student, University of Illinois at Urbana-Champaign (UIUC), U.S.A. (Advisor: Prof. Klaus Schulten)
09/2011-08/2015	B.S. in Chemistry (major), Computer Science (minor), Tsinghua University, P. R. China

PUBLICATIONS

1. **Hongde Yu**, Thomas Heine*. Magnetic Coupling Control in Triangulene Dimers. ***Journal of the American Chemical Society*** 2023, 145 (35), 19303-19311.
2. **Hongde Yu**, Jianwei Sun and Thomas Heine*. Predicting Magnetic Coupling and Spin-Polarization Energy in Triangulene Analogues. ***Journal of Chemical Theory and Computation*** 2023, 19 (12), 3486-3497.
3. **Hongde Yu**, Dong Wang*. Suppressing the Excitonic Effect in Covalent Organic Frameworks for Metal-Free Hydrogen Generation. ***JACS Au*** 2022, 2(8), 1848-1856. (**Cover**)
4. **Hongde Yu**, Dong Wang*. Metal-Free Magnetism in Chemically Doped Covalent Organic Frameworks. ***Journal of the American Chemical Society*** 2020, 142(25), 11013–11021. (Supplementary **Cover**)

5. **Hongde Yu**[#], Jinghui Wang[#], Liying Jiao and Dong Wang[*] *cis*-C=C Bond and Amide Regulated Oriented Supramolecular Assembly on Two-Dimensional Atomic Crystals. ***The Journal of Physical Chemistry C*** 2019, 123, 30996-31002.

6. Yamei Liu[#], Heng Zhang[#], **Hongde Yu**[#], Zhongquan Liao, Silvia Paasch, Shunqi Xu*, Ruyan Zhao, Eike Brunner, Mischa Bonn, Hai I Wang, Thomas Heine, Mingchao Wang*, Yiyong Mai*, Xinliang Feng*. ***Angewandte Chemie International Edition*** 2023, 62 (35), e202305978. **([#]equal contribution)**

7. Qingda Liu[#], **Hongde Yu**[#], Qinghua Zhang, Dong Wang* and Xun Wang*. Temperature-Responsive Self-Assembly of Single Polyoxometalates Clusters Driven by Hydrogen Bonds. ***Advanced Functional Materials***, 2021, 31, 2103561. **([#]equal contribution)**

8. Qingda Liu[#], Peilei He[#], **Hongde Yu**[#], Lin Gu, Bing Ni, Dong Wang[*] and Xun Wang[*] Single Molecule–Mediated Assembly of Polyoxometalate Single-Cluster Rings and Their Three-Dimensional Superstructures. ***Science Advances*** 2019, 5, eaax1081. **([#]equal contribution)**

9. Deren Yang[#], **Hongde Yu**[#], Ting He, Shouwei Zuo, Xiaozhi Liu, Haozhou Yang, Bing Ni, Haoyi Li, Lin Gu, Dong Wang and Xun Wang[*] Visible-Light-Switched Electron Transfer over Single Porphyrin-Metal Atom Center for Highly Selective Electroreduction of Carbon Dioxide. ***Nature Communications*** 2019, 10, 3844. **([#]equal contribution)**

10. Jinghui Wang[#], **Hongde Yu**[#], Xu Zhou, Xiaozhi Liu, Renjie Zhang, Zhixing Lu, Jingying Zhen, Lin Gu, Kaihui Liu, Dong Wang[*] and Liying Jiao[*] Probing the Crystallographic Orientation of Two-Dimensional Atomic Crystals with Supramolecular Self-Assembly. ***Nature Communications*** 2017, 8, 377. **([#]equal contribution)**

11. Dong Wang*, **Hongde Yu**[#], Wen Shi[#], Chunlin Xu. Chemical Doping of Organic and Coordination Polymers for Thermoelectric and Spintronic Applications: A Theoretical Understanding. ***Accounts of Chemical Research*** 2023, 56, 16, 2127–2138. **([#]equal contribution)**

12. Ruoyang Liu, Yongzhi Chen, **Hongde Yu**, Miroslav Polozij, Thomas Heine, Yuanyuan Guo, Tze Chien Sum, Donglin Jiang*. Linkage-engineered donor-acceptor covalent organic frameworks for optimal photosynthesis of hydrogen peroxide from water and air. ***Nature Catalysis***, 2024, 7, 195-206.

13. Yamei Liu, Qin Zhou, **Hongde Yu**, Qiqi Yang, Dr. Mingchao Wang, Chuanhui Huang, Luoxing Xiang, Chen Li, Thomas Heine, Guoqing Hu, Shengyao Wang, Xinliang Feng*, Yiyong Mai*. Increasing the Accessibility of Internal Catalytic Sites in Covalent Organic Frameworks by Introducing a Bicontinuous Mesostructure. ***Angewandte Chemie International Edition*** 2024, 136 (15), e202400985.

14. Yamei Liu, Mingchao Wang*, Changlin Dong, **Hongde Yu**, Yang Lu, Xing Huang, Silvia Paasch, Eike Brunner, Thomas Heine, Fang Song, Florian Auras, Fugui Xu*, Yiyong Mai, Xinliang Feng*. A thienyl-benzodithiophene-based two-dimensional conjugated covalent organic framework for fast photothermal conversion. ***Journal of Polymer Science*** 2023, 61 (16), 1843-1848.

15. Huili Ma, **Hongde Yu**, Qian Peng[*], Zhongfu An, Dong Wang and Zhigang Shuai[*] Hydrogen Bonding-Induced Morphology Dependence of Long-Lived Organic Room-Temperature Phosphorescence: A Computational Study. ***The Journal of Physical Chemistry Letters*** 2019, 10, 6948-6954.

16. Lifei Sun, Xingxu Yan, Jingying Zheng, **Hongde Yu**, Zhixing Lu, Shang-peng Gao, Lina Liu, Xiaoqing Pan, Dong Wang, Zhiguo Wang*, Peng Wang* and Liying Jiao* Layer-Dependent Chemically Induced Phase Transition of Two-Dimensional MoS_2. ***Nano Letters*** 2018, 18, 3435-3440.

17. Yuetong Kang, Xiaoyan Tang, **Hongde Yu**, Zhengguo Cai, Zehuan Huang, Dong Wang, Jiang-Fei Xu* and Xi Zhang* Supramolecular Catalyst Functions in Catalytic Amount: Cucurbit[8]uril Accelerates the Photodimerization of Brooker's Merocyanine. ***Chemical Science*** 2017, 8, 8357-8361.

18. Guangda Niu, **Hongde Yu**, Jiangwei, Li, Dong Wang and Liduo Wang* Controlled Orientation of Perovskite Films through Mixed Cations toward High Performance Perovskite Solar Cells. ***Nano Energy*** 2016, 27, 87-94.

19. Jun Xu, **Hongde Yu**, Liulin Yang, Guanglu Wu, Zhiqiang Wang, Dong Wang and Xi Zhang* Self-Assembling 1D Core/Shell Microrods by the Introduction of Additives: A One-Pot and Shell-Tunable Method. ***Chemical Science*** 2015, 6, 4907-4911.

PRESENTATIONS

1. High-throughput Prediction of Magnetic Covalent Organic Frameworks. *Summer School MATERIALS 4.0.* TU Dresden, Germany. (Online) 17/08/2020. (**Contributed talks**)

2. Theoretical studies of Supramolecular Assembly on MoS_2. *The 31st National Meeting of Chinese Chemical Society.* Hangzhou, P. R. China. 05/05/2018. (**Poster Award**)

3. Rational Design of Molecular Probes for Crystallographic Directions on 2D atomic Crystals. *The 16th International Congress of Quantum Chemistry (ICQC).* Menton, France. 18/06/2018. (Poster)

4. Theoretical Insights of Supramolecular Assembly on 2D Atomic Crystals. *11th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC).* Munich, Germany. 27/08/2017. (Poster)

HONORS AND AWARDS

15/10/2020	Tang Aoqing Chemistry Scholarship
15/10/2019	Tsinghua University Scholarship for Graduate Students, first-class
15/10/2018	Tsinghua University Future Scholar Scholarship
15/05/2018	Poster Award on the 31st National Meeting of Chinese Chemical Society
15/10/2017	Tsinghua University Scholarship for Graduate Students, second-class
15/10/2014	Tsinghua University Scholarship for Academic Excellence
2012-2014	Tsinghua Xuetang Talent Project Scholarship