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ACADEMIC PROFILES	My Google Scholar Record My Academic Genealogy	
EDUCATION	Ph.D. in Chemistry, <i>University of Pittsburgh</i> , Pittsburgh, PA • Adviser: Professor Kenneth Jordan	2007.08 – 2012.07
	M.Sc. in Physical Chemistry, <i>Fudan University</i> , Shanghai, China	2004.09 – 2007.06
	B.Sc. in Chemistry, <i>Wuhan University</i> , Wuhan, China	2000.09 – 2004.06
RESEARCH EXPERIENCES	Associate Research Fellow <i>University of Science and Technology of China</i> Single-atom catalysis, Photochemical conversion, Data-driven chemistry	2021.05 – present
	Research Associate <i>University of Science and Technology of China</i> Computational chemistry study on energy and materials conversion Machine learning protocol for spectroscopy simulation	2016.01 – 2021.04
	Postdoctoral Fellow Linda Broadbelt Group <i>Northwestern University</i> Quantum chemistry study of radical polymerization of methacrylate species	2012.08 – 2015.09
	Research Assistant Kenneth Jordan Group <i>University of Pittsburgh</i> Molecular modeling on methane hydrate Computational study on the water loading on a hydrophobic clay surface	2008.05 – 2012.07
	Research Assistant Kangnian Fan & Mingfei Zhou Group <i>Fudan University</i> Quantum chemistry study on the rare earth elements related chemical systems	2005.01 – 2007.06
ACADEMIC ACTIVITIES	Oral presentation The Spring 2021 ACS National Meeting (virtual meeting), USA The 32 th National Congress of Chemistry of Chinese Chemical Society, Zhuhai, China The 15 th National Conference on Computer Chemistry of China, Shanghai, China The Spring 2019 ACS National Meeting, Orlando, FL, USA The 31 th National Congress of Chemistry of Chinese Chemical Society, Hangzhou, China The 30 th National Congress of Chemistry of Chinese Chemical Society, Dalian, China	2021 2021 2019 2019 2018 2016
	Poster The 5 th International Symposium on Energy Chemistry and Materials, Shanghai, China (<i>Best Poster Reward</i>) The 16 th National Conference of Chemical Dynamics, Suzhou, China The 4 th International Symposium on Energy Chemistry and Materials, Xiamen, China The 14 th National Meeting of Quantum Chemistry, Dalian, China The 1 st International Symposium of New Molecules and Clusters, Shanghai, China	2019 2019 2018 2017 2016

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32. Ye, K.; Hu, M.; Li, Q.-K.; Luo, Y.; Jiang, J.; **Zhang, G.*** "Cooperative Single-Atom Active Centers for Attenuating the Linear Scaling Effect in the Nitrogen Reduction Reaction" *J. Phys. Chem. Lett.* 2021, 12, 5233-5240.
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30. Zhou, H.; He, F.; Chong, Y.; He, L.*; Jiang, J.; Luo, Y.; **Zhang, G.*** "Bridged Azobenzene Enables Dynamic Control of Through-Space Charge Transfer for Photochemical Conversion" *J. Phys. Chem. Lett.* 2021, 12, 3868-3974.
29. Chong, Y.; Zhang, X.; Chen, B.; Liu, R.; Wu, Z.; Zhang, G.; Jiang, J.; Mukamel S.; **Zhang, G.*** "Modulating Charge Separation and Intersystem Crossing in Donor-Switch-Acceptor Systems: A Computational Study" *J. Phys. Chem. A.* 2021, 125, 3088-3094.
28. Lv, S.; Li, X.; Yang, L.; Wang, X.; Zhang, J.; **Zhang, G.***; J. Jiang. "Azopyrazole-Based Photoswitchable Anion Receptor for Dihydrogen Phosphate Transport" *J. Phys. Chem. A.* 2020, 124, 9692-9697.
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25. Han, Y.; Li, Q-K.; Ye, K.; Luo, Y.; Jiang, J.; **Zhang, G.*** "Impact of Active Site Density on Oxygen Reduction Reactions Using Monodispersed Fe-N-C Single-Atom Catalysts" *ACS Appl. Mater. Interfaces.* 2020, 12, 15271-15278.
24. Xie, L.[†]; Zhu, Q.[†]; **Zhang, G.**[†]; Ye, K.; Zou, C.; Prezhdo, O. V.; Wang, Z.; Luo, Y.; Jiang, J. "Tunable Hydrogen Doping of Metal Oxide Semiconductors with Acid-Metal Treatment at Ambient Conditions" *J. Am. Chem. Soc.* 2020, 142, 4136-4140. (Co-first author)
23. Zhong, W.[†]; **Zhang, G.**[†]; Zhang, Y.; Jia, C.; Yang, T.; Ji, S.; Prezhdo, O.; Yuan, J.; Luo, Y.; Jiang, J. "Enhanced Activity of C₂N-Supported Single Co Atom Catalyst by Single Atom Promoter" *J. Phys. Chem. Lett.* 2019, 10, 7009-7014. (Co-first author)
22. Wu, Z.; Li, X.; Jiang, X.; Xie, T.; Li, H.; **Zhang, G.***; Jiang, J. "Photoswitchable De/Adsorption of Azobenzene-Derived Surfactant on Silica Surface" *Phys. Chem. Chem. Phys.* 2019, 21, 21030-21037.
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19. Yang, L.; Li, X.; Huang, Y.; Feng, S.; Wang, X.; Jiang, X.; Li, X.; Zhao, J.; **Zhang, G.***; Jiang, J. "Physically Close yet Chemically Separate Reduction and Oxidation Sites in Double-Walled Nanotubes for Photocatalytic Hydrogen Generation" *J. Phys. Chem. Lett.* 2019, 10, 3739-3743.
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9. Liu, X.-Y.[†]; **Zhang, G.**[†]; Chen, H.; Li, H.; Jiang, J.; Long, Y.-T.; Ning, Z. “Efficient defect-controlled photocatalytic hydrogen generation based on near-infrared Cu-In-Zn-S quantum dots” *Nano Research.* 2018, 11, 1379. (Co-first author)
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2. **Zhang, G.**; Al-Saidi, W. A.; Myshakin, E. M.; Jordan, K. D. “Dispersion-Corrected DFT and Classical Force Field Calculations of Water Loading on a Clay Surface” *J. Phys. Chem. C*. 2012, 116, 17134-17141.
1. **Zhang, G.**; Li, Z.; Wang, W.; Fan, K. “Decomposition of CH₂O by lanthanum: A theoretical study” *J. Phys. Chem. A*. 2007, 111, 11894-11903.

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2. Gong, Z. Y.; Duan, S.; Tian, G.; **Zhang, G.**; Jiang, J.; Luo, Y. "Optical Excitation in Donor-Pt-Acceptor Complexes: Role of the Structure." *J. Phys. Chem. A* 2016, 120, 3547-53.
1. Zheng, W.; **Zhang, G.**; Fan, K. "Synthesis and characterization of η^5 -1,2,4-diazaphospholide complexes of ruthenium." *Organometallics*. 2006, 25, 1548-1550.

PROFESSIONAL SKILLS

Computation Programs: Gaussian, VASP, ADF, Q-Chem, Turbomole, GROMACS, DL-POLY, LAMMPS
Programming Languages: Fortran 90, Python
Languages: Chinese (native), English (fluent)

HONORS

Outstanding Researcher of Year 2019 at University of Science and Technology of China
Excellent Researcher of Year 2018 at University of Science and Technology of China

2020
2019