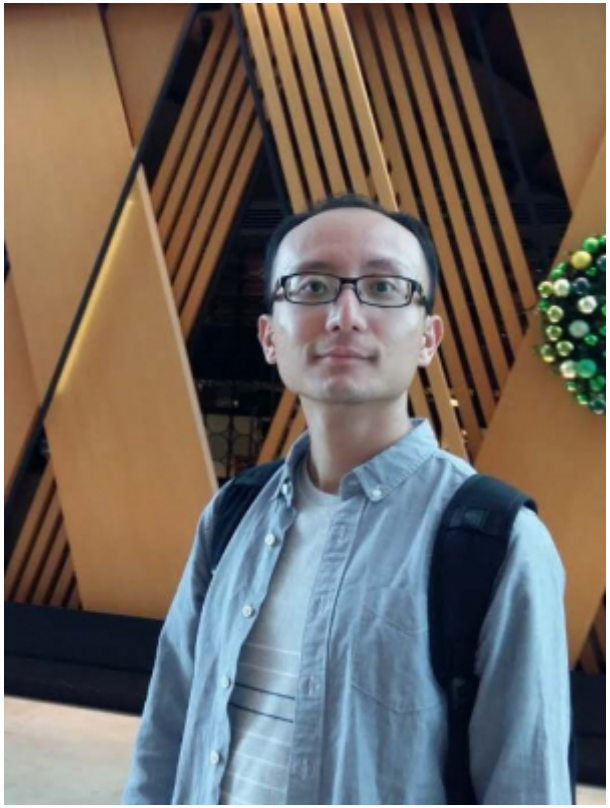
中山大學 化学学院
SUN YAT-SEN UNIVERSITY School of Chemistry



石文

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基本情况

姓名：石文

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出生年月：1989.10

出生地：新疆乌鲁木齐市

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教育经历

2012年8月–2017年7月，清华大学，化学系，化学专业博士学位（导师：帅志刚教授，王冬教授）

2008年9月–2012年7月，中国农业大学，理学院化学系，化学理科基地班，化学专业学士学位

工作经历

2021年3月—现在，中山大学化学学院，副教授

2017年9月—2021年2月，新加坡科技研究局（Agency for Science, Technology and Research，A*STAR），高性能计算研究所（Institute of High Performance Computing，IHPC），材料科学与化学系，Scientist

科研方向

理论与计算化学，材料计算与模拟

主要研究内容

1. 有机材料、有机−无机杂化材料、二维材料、共价有机框架和金属−有机框架中电、热输运的理论计算和模拟
2. 面向热电能源转化材料（包括有机分子热电材料、聚合物热电材料、杂化热电材料等），理论计算方法的发展和计算材料设计
3. 高通量计算在材料筛选和设计中的应用

欢迎有志于从事理论和计算化学，材料计算和模拟的优秀学子报考；欢迎具有研究热情的本科生加入开展科学探索工作；课题组长期招聘博士后。

科研项目

国家自然科学基金青年科学基金项目，24.0万，2022—2024，项目负责人

中山大学“百人计划”科研启动基金，30.0万，2021—2024，项目负责人

获奖情况

2019年5月，2018年度新加坡高性能计算研究所最佳文章奖

2017年7月，清华大学优秀博士学位论文二等奖

2016年10月，清华大学国家奖学金

2015年10月，清华大学综合优秀奖学金

2015年6月，第十五届国际量子化学大会最佳墙报奖

2014年10月，清华之友—陶氏化学一等奖学金

学术专著

《有机光电材料理论与计算》，帅志刚主编，“第8章：有机热电材料的理论研究进展”，王冬，**石文**，帅志刚，北京，科学出版社，“十三五”国家重点出版物出版规划项目，光电子科学与技术前沿丛书，2020。

学术论文

1. **Wen Shi**, Tianqi Deng, Zicong Marvin Wong, Gang Wu*, Shuo-Wang Yang*, “A Molecular Roadmap Towards Organic Donor-Acceptor Complexes with High-Performance Thermoelectric Response.” **npj Comput. Mater. 2021**, 7, 157.
2. Tianqi Deng, **Wen Shi**, Zicong Wong, Gang Wu*, Xiaoping Yang, Jin-Cheng Zheng, Hui Pan, Shuo-Wang Yang*, “Designing Intrinsic Topological Insulators in Two-Dimensional Metal-Organic Frameworks.” **J. Phys. Chem. Lett. 2021**, 12, 29, 6934.

3. Anqi Lv, Ze Yu, Yufeng Mao, Xiaoyan Zheng, **Wen Shi**, Huifang Shi, Wei Yao, Huili Ma*, Zhongfu An, "Molecular Conformation Dependence of Phosphorescence Lifetime in Organic Aggregates." **Dyes and Pigments 2021**, 193, 109520.
4. Tianqi Deng, Gang Wu*, **Wen Shi**, Zicong Marvin Wong, Jian-Sheng Wang, Shuo-Wang Yang*, "Ab Initio Dipolar Electron-Phonon Interactions in Two-Dimensional Materials." **Phys. Rev. B 2021**, 103, 075410.
5. **Wen Shi**, Zicong Marvin Wong, Tianqi Deng, Gang Wu*, Shuo-Wang Yang*, "Molecular Origin of Organic Semiconductors with High-Performance Thermoelectric Response." **Adv. Funct. Mater. 2021**, 31, 2007438.
6. Xue Yong, Gang Wu*, **Wen Shi**, Zicong Marvin Wong, Tianqi Deng, Qiang Zhu, Xiaoping Yang, Jian-Sheng Wang, Jianwei Xu, Shuo-Wang Yang*, "Theoretical Search for High-Performance Thermoelectric Donor-Acceptor Copolymers: The Role of Super-Exchange Couplings." **J. Mater. Chem. A 2020**, 8, 21852.
7. Zicong Marvin Wong, Tianqi Deng, **Wen Shi**, Gang Wu*, Shuo-Wang Yang*, "Strain Effects on the n-Type Thermoelectric Performance of Small-Molecule Organic Semiconductor 2-5-Difluoro-7,7,8,8-Tetracyanoquinodimethane." **ACS Appl. Energy Mater. 2020**, 3, 10174.
8. Xinyi Chen, **Wen Shi**, Kun Zhang*, "Observation of Energy-Dependent Carrier Scattering in Conducting Polymer Nanowires Blends for Enhanced Thermoelectric Performance." **ACS Appl. Mater. Interfaces 2020**, 12, 34451.
9. Zicong Marvin Wong, Tianqi Deng, **Wen Shi**, Gang Wu, Teck Leong Tan*, Shuo-Wang Yang*, "High Performance Photocatalytic and Thermoelectric Two-Dimensional Asymmetrically Ordered Janus-like MXene Alloy." **Mater. Adv. 2020**, 1, 1176.

10. **Wen Shi**, Erol Yildirim, Gang Wu, Zicong Marvin Wong, Tianqi Deng, Jian-Sheng Wang, Jianwei Xu, Shuo-Wang Yang*, "The Role of Electrostatic Interaction between Free Charge Carriers and Counterions in Thermoelectric Power Factor of Conducting Polymers: from Crystalline to Polycrystalline Domains." **Adv. Theory Simul. 2020**, 3, 2000015.（封底）
11. Anas Abutaha#, Pawan Kumar#, Erol Yildirim#, **Wen Shi**, Shuo-Wang Yang, Gang Wu*, Kedar Hippalgaonkar*, "Correlating Charge and Thermoelectric Transport to Paracrystallinity in Conducting Polymers." **Nat. Commun. 2020**, 11, 1737.
12. Tianqi Deng, Yong Xue, **Wen Shi**, Zicong Marvin Wong, Gang Wu, Hui Pan, Jian-Sheng Wang, Shuo-Wang Yang*, "Beyond Mahan-Sofo Best Thermoelectric: High Thermoelectric Performance from Directional π-Conjugation in Two-Dimensional Poly(tetrathienoanthracene)." **J. Mater. Chem. A 2020**, 8, 4257.
13. **Wen Shi**, Tianqi Deng, Gang Wu, Kedar Hippalgaonkar*, Jian-Sheng Wang, Shuo-Wang Yang*, "Unprecedented Enhancement of Thermoelectric Power Factor Induced by Pressure in Small-Molecule Organic Semiconductors." **Adv. Mater. 2019**, 31, 1901956.
14. **Wen Shi**, Dong Wang*, Zhigang Shuai*, "High-Performance Organic Thermoelectric Materials: Theoretical Insights and Computational Design." **Adv. Electron. Mater. 2019**, 5, 1800882.（综述）
15. Yunpeng Liu, **Wen Shi**, Tianqi Zhao, Dong Wang*, Zhigang Shuai*, "Boosting the Seebeck Coefficient for Organic Coordination Polymers: Role of Doping-Induced Polaron Band Formation." **J. Phys. Chem. Lett. 2019**, 10, 2493.
16. Tianqi Deng, Xue Yong, **Wen Shi**, Chee Kwan Gan, Wu Li, Kedar Hippalgaonkar, Jin-Cheng Zheng, Xiaobai Wang, Shuo-Wang Yang, Jian-Sheng Wang, Gang Wu*, "Two-Dimensional

Single-Layer π-Conjugated Nickel Bis(dithiolene) Complex: A Good-Electron-Poor-Phonon Thermoelectric Material." **Adv. Electron. Mater. 2019**, 5, 1800892.

17. Tian Zhang, **Wen Shi**, Dong Wang, Shuping Zhuo, Qian Peng*, Zhigang Shuai*, "Pressure-Induced Emission Enhancement in Hexaphenylsilole: A Computational Study." **J. Mater. Chem. C 2019**, 7, 1388.
18. **Wen Shi**, Gang Wu, Kedar Hippalgaonkar, Jian-Sheng Wang, Jianwei Xu, Shuo-Wang Yang*, "Poly(nickel-ethylenetetrathiolate) and Its Analogs: Theoretical Prediction of High-Performance Doping-Free Thermoelectric Polymers." **J. Am. Chem. Soc. 2018**, 140, 13200.
19. **Wen Shi**, Gang Wu, Xue Yong, Tianqi Deng, Jian-Sheng Wang, Jin-Cheng Zheng, Jianwei Xu, Michael B. Sullivan, Shuo-Wang Yang*, "Orbital-Engineering-Based Screening of π-Conjugated d8 Transition-Metal Coordination Polymers for High-Performance n-Type Thermoelectric Applications." **ACS Appl. Mater. Interfaces 2018**, 10, 35306.
20. Xue Yong#, **Wen Shi#(共一)**, Gang Wu, Shermin S. Goh, Shiqiang Bai, Jianwei Xu, Jian-Sheng Wang, Shuo-Wang Yang*, "Tuning the Thermoelectric Performance of p-d Conjugated Nickel Coordination Polymers Through Metal-Ligand Frontier Molecular Orbital Alignment." **J. Mater. Chem. A 2018**, 6, 19757.
21. **Wen Shi**, Zhigang Shuai, Dong Wang*, "Tuning Thermal Transport in Chain-Oriented Conducting Polymers for Enhanced Thermoelectric Efficiency: A Computational Study." **Adv. Funct. Mater. 2017**, 27, 1702847.（内封底）
22. Jun Wang, **Wen Shi**, Di Liu, Zijian Zhang, Yongfa Zhu*, Dong Wang*, "Supramolecular Organic Nanofibers with Highly Efficient and Stable Visible Light Photooxidation Performance." **Appl. Catal. B Environ. 2017**, 202, 289.

23. Jianfeng Chen, **Wen Shi**, Yuqian Jiang, Dong Wang*, Zhigang Shuai*, "Strain Induced Polymorphism and Band Structure Modulation in Low-Temperature 2,7-Dioctyl[1]benzothieno[3,2-b][1]benzothiophene Single Crystal." **Sci. China Chem. 2017**, 60, 275.

24. Yuma Nakamura, Tianqi Zhao, Jinyang Xi, **Wen Shi**, Dong Wang*, Zhigang Shuai*, "Intrinsic Charge Transport in Stanene: Roles of Bucklings and Electron-Phonon Couplings." **Adv. Electron. Mater. 2017**, 3, 1700143.

25. Huili Ma, **Wen Shi**, Jiajun Ren, Wenqiang Li, Qian Peng*, Zhigang Shuai*, "Electrostatic Interaction-Induced Room-Temperature Phosphorescence in Pure Organic Molecules from QM/MM Calculations." **J. Phys. Chem. Lett. 2016**, 7, 2893.

26. Tianqi Zhao, **Wen Shi**, Jinyang Xi, Dong Wang*, Zhigang Shuai*, "Intrinsic and Extrinsic Charge Transport in CH3NH3PbI3 Perovskites Predicted from First-Principles." **Sci. Rep. 2016**, 7, 19968.

27. Yuqian Jiang, Xinxin Zhong, **Wen Shi**, Qian Peng, Hua Geng, Yi Zhao*, Zhigang Shuai*, "Nuclear Quantum Tunnelling and Carrier Delocalization Effects to Bridge the Gap Between Hopping and Bandlike Behaviors in Organic Semiconductors." **Nanoscale Horiz. 2016**, 1, 53.（封底）

28. **Wen Shi**, Tianqi Zhao, Jinyang Xi, Dong Wang*, Zhigang Shuai*, "Unravelling Doping Effects on PEDOT at the Molecular Level: From Geometry to Thermoelectric Transport Properties." **J. Am. Chem. Soc. 2015**, 137, 12929.

29. **Wen Shi**, Jianming Chen, Jinyang Xi, Dong Wang*, Zhigang Shuai*, "Search for Organic Thermoelectric Materials with High Mobility: The Case of 2,7-Dialkyl[1]benzothieno[3,2-b][1]benzothiophene Derivatives." **Chem. Mater. 2014**, 26, 2669.

30. Yuqian Jiang, Hua Geng, **Wen Shi**, Qian Peng, Xiaoyan Zheng, Zhigang Shuai*, "Theoretical Prediction of Isotope Effects on Charge Transport in Organic Semiconductors." **J. Phys. Chem. Lett. 2014**, 5, 2267.
31. Dong Wang, **Wen Shi**, Jianming Chen, Jinyang Xi, Zhigang Shuai*, "Modeling Thermoelectric Transport in Organic Materials." **Phys. Chem. Chem. Phys. 2012**, 14, 16505.（封面综述）

学术报告

1. 2021年6月，The 4th International Symposium on Molecular Design of Opto-Electronic Materials. "A Molecular Roadmap Towards Organic Semiconductors with Increased Thermoelectric Response."（北京）（邀请报告）
2. 2019年6月，10th International Conference on Materials for Advanced Technologies, "Theoretical Investigations of the Pressure Effect on the Thermoelectric Properties in Small-Molecule Organic Semiconductors."（新加坡）（口头报告）
3. 2019年6月，Workshop on Electronic Materials and Devices 2019. "Computational Design of High-Performance Organic-Based Thermoelectric Materials."（香港大学）（邀请报告）
4. 2015年9月，Tsinghua–Bristol Symposium on Frontiers of Supramolecular Science. "Unravelling Doping Effects on PEDOT at the Molecular Level: from Geometry to Thermoelectric Transport Properties."（清华大学）（口头报告）