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科研方向

- 开发用于大尺度材料模拟的第一性原理电子结构计算方法和软件
- 开发材料结构预测方法和软件
- 基于密度泛函理论研究材料的物理和化学特性

教育经历

2013.09 – 2019.06 **吉林大学超硬材料国家重点实验室** **凝聚态物理 博士**

2009.09 – 2013.07 **吉林大学物理学院** **应用物理 本科**

科研经历

2019.09 – 现在 **美国罗格斯大学物理学院 博士后** **导师：Michele Pavanello**

- 机器学习：基于单电子约化密度矩阵开发了机器学习电子结构计算方法。
- 子系统密度泛函理论：发展了新的密度嵌入方法和方案。基于子系统密度泛函理论开发了 Python 软件 eDFTpy。
- 无轨道密度泛函理论：发展了高效的无轨道密度泛函理论求解器和非局域动能泛函。基于密度泛函理论开发了 Python 软件 DFTpy。

2013.09 – 2019.06 **吉林大学超硬材料国家重点实验室 博士** **导师：马琰铭**

- 发展晶体结构预测方法并参与开发和维护 CALYPSO 软件包。
- 开发了 ATLAS 方法和软件包，以促进无轨道密度泛函理论在大尺度材料模拟中的广泛使用。

学术活动

2023.03	主持人	APS 2023 年三月会议	Density Functional Theory in Chemical Physics III
2023.03	报告	APS 2023 年三月会议	Ab-initio Adaptive Density Embedding for Mesoscale Systems
2022.03	报告	APS 2022 年三月会议	DFT Embedding in Python for Realistically-sized Systems
2021.03	报告	APS 2021 年三月会议	An Efficient DFT Solver for Nanoscale Simulations and Beyond
2020.08	报告	ACS 2020 年秋季会议	DFTpy: An efficient and object-oriented platform for orbital-free DFT simulations
2018.10	报告	第六届 CALYPSO 研讨会	ATLAS: A real-space finite-difference implementation of orbital-free density functional theory
2017.10	报告	第五届 CALYPSO 研讨会	The advanced mode of CALYPSO for structure prediction
2016.06	海报	第九届计算纳米科学与新能源材料国际研讨会	ATLAS: A real-space finite-difference implementation of orbital-free density functional theory

荣誉奖项

2023 优秀博士后奖 美国罗格斯大学物理学院

2020	MolSSI 软件奖学金	美国分子科学软件研究所（MolSSI）
2020	Wiley 计算机化学杰出博士后奖	美国化学学会（ACS）
2016	优秀青年海报奖	第九届计算纳米科学与新能源材料国际研讨会
2014	研究生国家奖学金	中华人民共和国教育部

发表文章

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1 X. Shao†, L. Paetow, M. E. Tuckerman†, and M. Pavanello†, "Machine Learning Electronic Structure Methods Based On The One-Electron Reduced Density Matrix", Nature Communications 14, 6281 (2023).

2 X. Shao†, A. C. Lopez, M. R. Khan Musa, M. R. Nouri, and M. Pavanello†, "Adaptive Subsystem Density Functional Theory", Journal of Chemical Theory and Computation 18, 6646–6655 (2022).

3 X. Shao†, W. Mi†, and M. Pavanello†, "Density Embedding Method for Nanoscale Molecule–Metal Interfaces", The Journal of Physical Chemistry Letters 13, 7147–7154 (2022).

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5 X. Shao†, A. Umerbekova, K. Jiang, and M. Pavanello†, "Many-body van der Waals interactions in wet MoS2 surfaces", Electronic Structure 4, 024001 (2022).

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9 X. Shao, K. Jiang, W. Mi, A. Genova, and M. Pavanello, "DFTpy: An efficient and object-oriented platform for orbital-free DFT simulations", Wiley Interdisciplinary Reviews: Computational Molecular Science 11, e1482 (2021).

10 X. Shao, X. Qu, S. Liu, L. Yang, J. Yang, X. Liu, X. Zhong, S. Sun, G. Vaitheeswaran, and J. Lv, "Structure evolution of chromium-doped boron clusters: toward the formation of endohedral boron cages", RSC Advances 9, 2870–2876 (2019).

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12 X. Shao*, W. Mi*, Q. Xu, Y. Wang, and Y. Ma, "O(NlogN) scaling method to evaluate the ion–electron potential of crystalline solids", The Journal of Chemical Physics 145, 184110 (2016).

13 Z. A. Moldabekov†, X. Shao†, M. Pavanello†, J. Vorberger, F. Graziani, and T. Dornheim, "Imposing correct jellium response is key to predict the density response by orbital-free DFT", Physical Review B 108, 235168 (2023).

14 J. A. Martinez B, L. Paetow, J. Tolle,¨ X. Shao†, P. Ramos, J. Neugebauer†, and M. Pavanello†, "Which Physical Phenomena Determine the Ionization Potential of Liquid Water?", The Journal of Physical Chemistry. B 127, 5470–5480 (2023).

[15] L. Fiedler†, Z. A. Moldabekov†, X. Shao†, K. Jiang†, T. Dornheim†, M. Pavanello†, and A. Cangi†, "Accelerating equilibration in first-principles molecular dynamics with orbital-free density functional theory", Physical Review Research 4, 043033 (2022).

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