Xuecheng Shao

Curriculum Vitae

Personal Details

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Research Interests

- Development of electronic structure methods and software for large-scale ab-initio materials simulations.
- Development of complex crystal structure prediction methods and software.
- Materials simulation based on density functional theory.
- Investigating the physical and chemical properties of materials.
- Pushing the limits of Python for scientific programming.

Education

9/2013–6/2019	Ph.D. in Condensed Matter Physics, State Key Lab of Superhard Materials, Jilin University, Changchun, China
9/2009–7/2013	B.S. in Physics, Department of Physics, Jilin University, Changchun, China

Research Experience

9/2019–present Postdoc Advisor: Professor Michele Pavanello

- Machine learning: Developed surrogate electronic structure methods based on machine learning of the one-electron reduced density matrix.
- Density embedding (methods and software): Developed new density embedding methods and schemes for density embedding simulations. Developed a Python software eDFTpy.
- Orbital-free density functional theory (methods and software): Developed an efficient DFT solver and nonlocal kinetic energy functional for large-scale simulations. Developed a Python software DFTpy.

9/2013–7/2019 Graduate Advisor: Professor Yanming Ma

- Development of crystal structure prediction methods and software package CALYPSO.
- Development of new methods and software package ATLAS for promoting the extensive use of OF-DFT for large-scale simulations.

Scientific Activities

- 03/2023 Chair APS March Meeting 2023, “Density Functional Theory in Chemical Physics III”
- 03/2023 Talk APS March Meeting 2023, “Ab-initio Adaptive Density Embedding for Mesoscale Systems”
- 03/2022 Talk APS March Meeting 2022, “DFT Embedding in Python for Realistically-sized Systems”

- 03/2021 Talk APS March Meeting 2021, "An Efficient DFT Solver for Nanoscale Simulations and Beyond"
- 08/2020 Talk ACS Fall 2020 VIRTUAL Meeting & Expo, "DFTpy: An efficient and object-oriented platform for orbital-free DFT simulations"
- 10/2018 Talk 6th CALYPSO workshop, Xi'an, China, "ATLAS: A real-space finite-difference implementation of orbital-free density functional theory"
- 10/2017 Talk 5th CALYPSO workshop, Changchun, China, "The advanced mode of CALYPSO for structure prediction"
- 10/2016 Talk 4th CALYPSO workshop, Nanjing, China, "The advanced mode of CALYPSO for structure prediction"
- 06/2016 Poster 9th International Conference on Computational Nanoscience and New Energy Materials, Shanghai, China, "ATLAS: A real-space finite-difference implementation of orbital-free density functional theory"

Awards

- 2023 Postdoctoral Excellence Award, Physics Department Rutgers University-Newark
- 2020 MolSSI Software Fellow
- 2020 Wiley Computers in Chemistry Outstanding Postdoc Award
- 2016 Excellent Young Poster Award, the 9th International Conference on Computational Nanoscience and New Energy Materials
- 2014 National Scholarship, Ministry of Education, China

Publications

* indicates equal contributions
† indicates corresponding author(s)

[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).

[4] **X. Shao***, J. Lv*, P. Liu, S. Shao, P. Gao, H. Liu, Y. Wang, and Y. Ma, "A symmetry-orientated divide-and-conquer method for crystal structure prediction", The Journal of Chemical Physics **156**, 014105 (2022).

[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).

[6] **X. Shao**, W. Mi, and M. Pavanello, "Revised Huang-Carter nonlocal kinetic energy functional for semiconductors and their surfaces", Physical Review B **104**, 045118 (2021).

[7] **X. Shao**, W. Mi, and M. Pavanello, "GGA-Level Subsystem DFT Achieves Sub-kcal/mol Accuracy Intermolecular Interactions by Mimicking Nonlocal Functionals", Journal of Chemical Theory and Computation **17**, 3455–3461 (2021).

[8] **X. Shao**, W. Mi, and M. Pavanello, "Efficient DFT Solver for Nanoscale Simulations and Beyond", The Journal of Physical Chemistry Letters **12**, 4134–4139 (2021).

[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).

[11] **X. Shao**, Q. Xu, S. Wang, J. Lv, Y. Wang, and Y. Ma, "Large-scale ab initio simulations for periodic system", Computer Physics Communications **233**, 78–83 (2018).

[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. Tölle, **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).

[16] K. Jiang[†], **X. Shao**[†], and M. Pavanello[†], "Efficient time-dependent orbital-free density functional theory: Semilocal adiabatic response", Physical Review B **106**, 115153 (2022).

[17] K. Jiang[†], **X. Shao**[†], and M. Pavanello[†], "Nonlocal and nonadiabatic Pauli potential for time-dependent orbital-free density functional theory", Physical Review B **104**, 235110 (2021).

[18] W. Mi[†], **X. Shao**[†], A. Genova[†], D. Ceresoli[†], and M. Pavanello[†], "eQE 2.0: Subsystem DFT Beyond GGA Functionals", Computer Physics Communications **269**, 108122 (2021).

[19] W. Mi[*], **X. Shao**[*], C. Su, Y. Zhou, S. Zhang, Q. Li, H. Wang, L. Zhang, M. Miao, Y. Wang, et al., "ATLAS: A real-space finite-difference implementation of orbital-free density functional theory", Computer Physics Communications **200**, 87–95 (2016).

[20] J. A. Martinez B, **X. Shao**, K. Jiang, and M. Pavanello, "Entropy is a good approximation to the electronic (static) correlation energy", The Journal of Chemical Physics **159**, 191102 (2023).

[21] Z. Moldabekov, S. Schwalbe, M. P. Böhme, J. Vorberger, **X. Shao**, M. Pavanello, F. R. Graziani, and T. Dornheim, "Bound-State Breaking and the Importance of Thermal Exchange–Correlation Effects in Warm Dense Hydrogen", Journal of Chemical Theory and Computation **20**, 68–78 (2024).

[22] W. Gong, R. Xu, **X. Shao**, Q. Li, and C. Chen, "Stability and mechanical properties of $W_{1-x}Mo_xB_{4.2}$ ($x = 0.0 - 1.0$) from first principles", Physical Review Materials **5**, 123606 (2021).

[23] Y. Wang, M. Xu, L. Yang, B. Yan, Q. Qin, **X. Shao**, Y. Zhang, D. Huang, X. Lin, J. Lv, et al., "Pressure-stabilized divalent ozonide CaO3 and its impact on Earth's oxygen cycles", Nature Communications **11**, 4702 (2020).

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[25] K. Yin, P. Gao, **X. Shao**, B. Gao, H. Liu, J. Lv, S. T. John, Y. Wang, and Y. Ma, "An automated predictor for identifying transition states in solids", npj Computational Materials **6**, 16 (2020).

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[27] S. Deng, X. Song, **X. Shao**, Q. Li, Y. Xie, C. Chen, and Y. Ma, "First-principles study of high-pressure phase stability and superconductivity of Bi_4I_4", Physical Review B **100**, 224108 (2019).

[28] P. Jiang, Z. Lei, L. Chen, **X. Shao**, X. Liang, J. Zhang, Y. Wang, J. Zhang, Z. Liu, and J. Feng, "Polyethylene Glycol–Na+ Interface of Vanadium Hexacyanoferrate Cathode for Highly Stable Rechargeable Aqueous Sodium-Ion Battery", ACS Applied Materials & Interfaces **11**, 28762–28768 (2019).

[29] J. Wang, X. Song, **X. Shao**, B. Gao, Q. Li, and Y. Ma, "High-Pressure Evolution of Unexpected Chemical Bonding and Promising Superconducting Properties of YB6", The Journal of Physical Chemistry C **122**, 27820–27828 (2018).

[30] J. Lv, M. Xu, S. Lin, **X. Shao**, X. Zhang, Y. Liu, Y. Wang, Z. Chen, and Y. Ma, "Direct-gap semiconducting tri-layer silicene with 29% photovoltaic efficiency", Nano Energy **51**, 489–495 (2018).

[31] Y. Zhang, **X. Shao**, Y. Zheng, L. Yan, P. Zhu, Y. Li, and H. Xu, "Pressure-induced structural transitions and electronic topological transition of Cu2Se", Journal of Alloys and Compounds **732**, 280–285 (2018).