

## Personal Details

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Web <http://www.shaoxc.com>  
Mail [sxc@calypso.cn](mailto:sxc@calypso.cn) / [shao\\_xc@163.com](mailto:shao_xc@163.com) / [xuecheng.shao@rutgers.edu](mailto:xuecheng.shao@rutgers.edu)  
Address Department of Physics, Rutgers University, 101 Warren Street, Newark, NJ 07102, USA

## Research Interests

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- 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

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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

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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

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- 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

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- 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

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\* indicates equal contributions

† indicates corresponding author(s)

- <sup>1</sup> [X. Shao](#)<sup>†</sup>, L. Paetow, M. E. Tuckerman<sup>†</sup>, and M. Pavanello<sup>†</sup>, “Machine Learning Electronic Structure Methods Based On The One-Electron Reduced Density Matrix”, [Nature Communications](#) **14**, 6281 (2023).
- <sup>2</sup> [X. Shao](#)<sup>†</sup>, A. C. Lopez, M. R. Khan Musa, M. R. Nouri, and M. Pavanello<sup>†</sup>, “Adaptive Subsystem Density Functional Theory”, [Journal of Chemical Theory and Computation](#) **18**, 6646–6655 (2022).
- <sup>3</sup> [X. Shao](#)<sup>†</sup>, W. Mi<sup>†</sup>, and M. Pavanello<sup>†</sup>, “Density Embedding Method for Nanoscale Molecule–Metal Interfaces”, [The Journal of Physical Chemistry Letters](#) **13**, 7147–7154 (2022).
- <sup>4</sup> [X. Shao](#)<sup>\*</sup>, J. Lv<sup>\*</sup>, 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).
- <sup>5</sup> [X. Shao](#)<sup>†</sup>, A. Umerbekova, K. Jiang, and M. Pavanello<sup>†</sup>, “Many-body van der Waals interactions in wet MoS<sub>2</sub> surfaces”, [Electronic Structure](#) **4**, 024001 (2022).
- <sup>6</sup> [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).
- <sup>7</sup> [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).
- <sup>8</sup> [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).
- <sup>9</sup> [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).
- <sup>10</sup> [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).

- <sup>11</sup> 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).
- <sup>12</sup> 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).
- <sup>13</sup> 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).
- <sup>14</sup> 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).
- <sup>15</sup> 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).
- <sup>16</sup> 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).
- <sup>17</sup> K. Jiang†, X. Shao†, and M. Pavanello†, “Efficient time-dependent orbital-free density functional theory: Semilocal adiabatic response”, *Physical Review B* **106**, 115153 (2022).
- <sup>18</sup> 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).
- <sup>19</sup> 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).
- <sup>20</sup> 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).
- <sup>21</sup> S. Tao, X. Shao, and L. Zhu, “Accelerating Structural Optimization through Fingerprinting Space Integration on the Potential Energy Surface”, *The Journal of Physical Chemistry Letters* **15**, 3185–3190 (2024).
- <sup>22</sup> 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).
- <sup>23</sup> 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).
- <sup>24</sup> 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  $CaO_3$  and its impact on Earth’s oxygen cycles”, *Nature Communications* **11**, 4702 (2020).
- <sup>25</sup> Z. Wang, D. Wang, Z. Zou, T. Song, D. Ni, Z. Li, X. Shao, W. Yin, Y. Wang, W. Luo, et al., “Efficient potential-tuning strategy through p-type doping for designing cathodes with ultrahigh energy density”, *National Science Review* **7**, 1768–1775 (2020).
- <sup>26</sup> 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).
- <sup>27</sup> Q. Xu, S. Wang, L. Xue, X. Shao, P. Gao, J. Lv, Y. Wang, and Y. Ma, “Ab initio electronic structure calculations using a real-space Chebyshev-filtered subspace iteration method”, *Journal of Physics: Condensed Matter* **31**, 455901 (2019).
- <sup>28</sup> 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).
- <sup>29</sup> 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).
- <sup>30</sup> 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  $YB_6$ ”, *The Journal of Physical Chemistry C* **122**, 27820–27828 (2018).
- <sup>31</sup> 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).

<sup>32</sup> Y. Zhang, [X. Shao](#), Y. Zheng, L. Yan, P. Zhu, Y. Li, and H. Xu, “Pressure-induced structural transitions and electronic topological transition of Cu<sub>2</sub>Se”, [Journal of Alloys and Compounds](#) **732**, 280–285 (2018).