# Xuecheng Shao

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8241540/publications.pdf

Version: 2024-02-01

| | | | |
|---|---|---|---|
| 22 papers | 450 citations | 687220 13 h-index | 713332 21 g-index |
| 22 all docs | 22 docs citations | 22 times ranked | 502 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | A symmetry-orientated divide-and-conquer method for crystal structure prediction. Journal of Chemical Physics, 2022, 156, 014105. | 1.2 | 40 |
| 2 | Many-body van der Waals interactions in wet MoS<sub>2</sub> surfaces. Electronic Structure, 2022, 4, 024001. | 1.0 | 2 |
| 3 | <scp>DFTpy</scp>: An efficient and objectâ€oriented platform for orbitalâ€free <scp>DFT</scp> simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, . | 6.2 | 34 |
| 4 | Efficient DFT Solver for Nanoscale Simulations and Beyond. Journal of Physical Chemistry Letters, 2021, 12, 4134-4139. | 2.1 | 13 |
| 5 | GGA-Level Subsystem DFT Achieves Sub-kcal/mol Accuracy Intermolecular Interactions by Mimicking Nonlocal Functionals. Journal of Chemical Theory and Computation, 2021, 17, 3455-3461. | 2.3 | 9 |
| 6 | Revised Huang-Carter nonlocal kinetic energy functional for semiconductors and their surfaces. Physical Review B, 2021, 104, . | 1.1 | 15 |
| 7 | eQE 2.0: Subsystem DFT beyond GGA functionals. Computer Physics Communications, 2021, 269, 108122. | 3.0 | 13 |
| 8 | Stability and mechanical properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">W</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow><mml:mi mathvariant="normal">Mo</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mrow><mml:mn>4.2</mml:mn></mml:mrow></mml:msub></mml:math> | | |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Large-scale ab initio simulations for periodic system. Computer Physics Communications, 2018, 233, 78-83. | 3.0 | 23 |
| 20 | O ( N log N ) scaling method to evaluate the ionâ€“electron potential of crystalline solids. Journal of Chemical Physics, 2016, 145, 184110. | 1.2 | 7 |
| 21 | ATLAS: A real-space finite-difference implementation of orbital-free density functional theory. Computer Physics Communications, 2016, 200, 87-95. | 3.0 | 42 |
| 22 | Electronic Topological Transition in Ag2Te at High-pressure. Scientific Reports, 2015, 5, 14681. | 1.6 | 20 |