Jinyang Xi

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	First-principles prediction of charge mobility in carbon and organic nanomaterials. Nanoscale, 2012, 4, 4348.	2.8	551
2	Carrier Mobility in Graphyne Should Be Even Larger than That in Graphene: A Theoretical Prediction. Journal of Physical Chemistry Letters, 2013, 4, 1443-1448.	2.1	328
3	Unravelling Doping Effects on PEDOT at the Molecular Level: From Geometry to Thermoelectric Transport Properties. Journal of the American Chemical Society, 2015, 137, 12929-12938.	6.6	176
4	Discovery of High-Performance Thermoelectric Chalcogenides through Reliable High-Throughput Material Screening. Journal of the American Chemical Society, 2018, 140, 10785-10793.	6.6	134
5	Intrinsic and Extrinsic Charge Transport in CH3NH3PbI3 Perovskites Predicted from First-Principles. Scientific Reports, 2016, 6, 19968.	1.6	119
6	Tunable Electronic Properties of Two-Dimensional Transition Metal Dichalcogenide Alloys: A First-Principles Prediction. Journal of Physical Chemistry Letters, 2014, 5, 285-291.	2.1	98
7	Modeling thermoelectric transport in organic materials. Physical Chemistry Chemical Physics, 2012, 14, 16505.	1.3	93
8	Electron-phonon couplings and carrier mobility in graphynes sheet calculated using the Wannier-interpolation approach. Journal of Chemical Physics, 2014, 141, 034704.	1.2	82
9	Achieving band convergence by tuning the bonding ionicity in nâ€ŧype Mg ₃ Sb ₂ . Journal of Computational Chemistry, 2019, 40, 1693-1700.	1.5	68
10	TransOpt. A code to solve electrical transport properties of semiconductors in constant electron–phonon coupling approximation. Computational Materials Science, 2021, 186, 110074.	1.4	55
11	Intrinsic Charge Transport in Stanene: Roles of Bucklings and Electron–Phonon Couplings. Advanced Electronic Materials, 2017, 3, 1700143.	2.6	47
12	Electronic properties and charge carrier mobilities of graphynes and graphdiynes from first principles. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 215-227.	6.2	42
13	Thermoelectric transport properties in chalcogenides ZnX (X=S, Se): From the role of electron-phonon couplings. Journal of Materiomics, 2021, 7, 310-319.	2.8	24
14	Temperature-dependent band gaps in several semiconductors: from the role of electron–phonon renormalization. Journal of Physics Condensed Matter, 2020, 32, 475503.	0.7	23
15	Theoretical Studies on the Deformation Potential, Electron-Phonon Coupling, and Carrier Transports of Layered Systems. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2018, 34, 961-976.	2.2	21
16	Strong electron-phonon interaction induced significant reduction in lattice thermal conductivities for single-layer MoS2 and PtSSe. Materials Today Physics, 2020, 15, 100277.	2.9	19
17	Temperature-dependence of the band gap in the all-inorganic perovskite CsPbI ₃ from room to high temperatures. Physical Chemistry Chemical Physics, 2022, 24, 16003-16010.	1.3	17
18	Temperature-Dependent Band Renormalization in CoSb ₃ Skutterudites Due to Sb-Ring-Related Vibrations. Chemistry of Materials, 2021, 33, 1046-1052.	3.2	16

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19	The origin of intrinsic charge transport for Dirac carbon sheet materials: roles of acetylenic linkage and electron–phonon couplings. Nanoscale, 2019, 11, 10828-10837.	2.8	12
20	Temperatureâ€dependent structural fluctuation and its effect on the electronic structure and charge transport in hybrid perovskite <scp>CH₃NH₃PbI₃</scp> . Journal of Computational Chemistry, 2021, 42, 2213-2220.	1.5	12
21	Unraveling the relationships between chemical bonding and thermoelectric properties: n-type ABO ₃ perovskites. Journal of Materials Chemistry A, 2022, 10, 11039-11045.	5.2	10
22	Accelerating the Discovery of Cu–Sn–S Thermoelectric Compounds via High-Throughput Synthesis, Characterization, and Machine Learning-Assisted Image Analysis. Chemistry of Materials, 2021, 33, 6918-6924.	3.2	8
23	Significant reduction in lattice thermal conductivity in a p-type filled skutterudite due to strong electron–phonon interactions. Journal of Materials Chemistry A, 2022, 10, 13484-13491.	5.2	8
24	Perspective of the electron–phonon interaction on the electrical transport in thermoelectric/electronic materials. Applied Physics Letters, 2022, 120, .	1.5	5
25	Mechanism of charge transport in organic semiconductors and carbon nanomaterials. Materials Research Society Symposia Proceedings, 2015, 1733, 1.	0.1	0