Haiyang Niu

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8640897/publications.pdf

Version: 2024-02-01

29 papers	3,498 citations	361045 20 h-index	476904 29 g-index
30 all docs	30 docs citations	30 times ranked	2751 citing authors

#	Article	IF	Citations
1	Modeling hardness of polycrystalline materials and bulk metallic glasses. Intermetallics, 2011, 19, 1275-1281.	1.8	1,811
2	Families of Superhard Crystalline Carbon Allotropes Constructed via Cold Compression of Graphite and Nanotubes. Physical Review Letters, 2012, 108, 135501.	2.9	167
3	Extra-electron induced covalent strengthening and generalization of intrinsic ductile-to-brittle criterion. Scientific Reports, 2012, 2, 718.	1.6	165
4	Structure, bonding, and possible superhardness of CrB<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 85, .	1.1	154
5	Hardness of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>T</mml:mi></mml:math>-carbon: Density functional theory calculations. Physical Review B, 2011, 84, .	1.1	140
6	Simple and accurate model of fracture toughness of solids. Journal of Applied Physics, 2019, 125, .	1.1	136
7	Ab initio phase diagram and nucleation of gallium. Nature Communications, 2020, 11, 2654.	5.8	102
8	Computational Prediction of Boron-Based MAX Phases and MXene Derivatives. Chemistry of Materials, 2020, 32, 6947-6957.	3.2	89
9	Pressure-stabilized hafnium nitrides and their properties. Physical Review B, 2017, 95, .	1.1	85
10	Molecular dynamics simulations of liquid silica crystallization. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 5348-5352.	3.3	78
11	Interstitial-boron solution strengthened WB3+x. Applied Physics Letters, 2013, 103, .	1.5	72
12	Electronic, optical, and mechanical properties of superhard cold-compressed phases of carbon. Applied Physics Letters, 2011, 99, .	1.5	68
13	Temperature Dependence of Homogeneous Nucleation in Ice. Physical Review Letters, 2019, 122, 245501.	2.9	56
14	Variable-composition structural optimization and experimental verification of MnB₃and MnB₄. Physical Chemistry Chemical Physics, 2014, 16, 15866-15873.	1.3	49
15	A combined molecular dynamics and experimental study of two-step process enabling low-temperature formation of phase-pure Î±-FAPbI ₃. Science Advances, 2021, 7, .	4.7	49
16	First-principles study of Zrâ€“N crystalline phases: phase stability, electronic and mechanical properties. RSC Advances, 2017, 7, 4697-4703.	1.7	45
17	Prediction of novel stable compounds in the Mg-Si-O system under exoplanet pressures. Scientific Reports, 2016, 5, 18347.	1.6	43
18	Improving collective variables: The case of crystallization. Journal of Chemical Physics, 2019, 150, 094509.	1.2	38

#	Article	IF	Citations
19	Diverse Chemistry of Stable Hydronitrogens, and Implications for Planetary and Materials Sciences. Scientific Reports, 2016, 6, 25947.	1.6	27
20	Combining Metadynamics and Integrated Tempering Sampling. Journal of Physical Chemistry Letters, 2018, 9, 6426-6430.	2.1	27
21	Atomic configurations of various kinds of structural intergrowth in the polytypic M2B-type boride precipitated in the Ni-based superalloy. Acta Materialia, 2015, 100, 64-72.	3.8	18
22	Superconductivity and unexpected chemistry of germanium hydrides under pressure. Physical Review B, 2017, 95, .	1.1	16
23	Vacancy formation enthalpy of filled<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>d</mml:mi></mml:math>-band noble metals by hybrid functionals. Physical Review B, 2014, 90, .	1.1	15
24	COPEX: co-evolutionary crystal structure prediction algorithm for complex systems. Npj Computational Materials, 2021, 7, .	3.5	13
25	A novel phase of beryllium fluoride at high pressure. Physical Chemistry Chemical Physics, 2015, 17, 26283-26288.	1.3	11
26	The system Taâ€“Vâ€“Si: Crystal structure and phase equilibria. Journal of Solid State Chemistry, 2012, 187, 114-123.	1.4	9
27	Tuning of electronic and optical properties of a predicted silicon allotrope: Hexagonal silicon <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>h</mml:mi><mml:mn>10</mml:mn></mml:mrow></mml -Si. Physical Review B, 2021, 104, .	1.1	7
28	The system Taâ€“Vâ€“Si: Thermodynamic modeling. Journal of Solid State Chemistry, 2013, 199, 171-180.	1.4	5
29	Unraveling the mechanisms of aluminum solidification under hyper-gravity condition from molecular dynamics simulations. Journal of Applied Physics, 2022, 132, .	1.1	3