Congwei Xie

List of Publications by Year
in descending order

18	479	686830 13	839053 18
papers	citations	h-index	g-index

18	18	18	755
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Prediction of Fluorooxoborates with Colossal Second Harmonic Generation (SHG) Coefficients and Extremely Wide Band Gaps: Towards Modulating Properties by Tuning the BO₃/BO₃F Ratio in Layers. Angewandte Chemie - International Edition, 2019, 58, 11726-11730.	7.2	66
2	New Tungsten Borides, Their Stability and Outstanding Mechanical Properties. Journal of Physical Chemistry Letters, 2018, 9, 3470-3477.	2.1	61
3	Computer-aided design of metal chalcohalide semiconductors: from chemical composition to crystal structure. Chemical Science, 2018, 9, 1022-1030.	3.7	54
4	Effects of carbon vacancies on the structures, mechanical properties, and chemical bonding of zirconium carbides: a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 12299-12306.	1.3	53
5	Prediction of stable hafnium carbides: Stoichiometries, mechanical properties, and electronic structure. Physical Review B, 2013, 88, .	1.1	51
6	Evolutionary search for new high-kdielectric materials: methodology and applications to hafnia-based oxides. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 76-84.	0.2	44
7	Novel high-pressure calcium carbonates. Physical Review B, 2018, 98, .	1.1	32
8	Monte Carlo simulation of polycrystalline microstructures and finite element stress analysis. Materials & Design, 2014, 55, 740-746.	5.1	18
9	Prediction of Fluorooxoborates with Colossal Second Harmonic Generation (SHG) Coefficients and Extremely Wide Band Gaps: Towards Modulating Properties by Tuning the BO₃/BO₃F Ratio in Layers. Angewandte Chemie, 2019, 131, 11852-11856.	1.6	16
10	First-principles calculations of the dielectric and vibrational properties of ferroelectric and paraelectric BaAl2O4. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 1867-1870.	0.9	15
11	Rational design of inorganic dielectric materials with expected permittivity. Scientific Reports, 2015, 5, 16769.	1.6	14
12	Stressed oxidation life predication of 3D C/SiC composites in a combustion wind tunnel. Composites Science and Technology, 2013, 88, 178-183.	3.8	13
13	Stable and hard hafnium borides: A first-principles study. Journal of Applied Physics, 2019, 125, .	1.1	13
14	Discovering novel VC1â‾' compounds through hybrid first-principles and evolutionary algorithms. Journal of the European Ceramic Society, 2016, 36, 3593-3599.	2.8	10
15	Revealing the Potential Crystal Structures of Earth-Abundant Nontoxic Photovoltaic CuBiI₄. Crystal Growth and Design, 2021, 21, 2850-2855.	1.4	8
16	Discovering low-permittivity materials: Evolutionary search for MgAl2O4 polymorphs. Applied Physics Letters, 2014, 105, .	1.5	4
17	High-pressure structure prediction of Hf-C system and first-principle simulation of their electronic properties. Wuli Xuebao/Acta Physica Sinica, 2015, 64, 236102.	0.2	4
18	Revealing the crystal structures and relative dielectric constants of fluorinated silicon oxides. Journal of Materials Chemistry C, 2021, 9, 15983-15989.	2.7	3