

# Congwei Xie

## List of Publications by Year in descending order

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18  
papers

479  
citations

687363  
13  
h-index

839539  
18  
g-index

18  
all docs

18  
docs citations

18  
times ranked

755  
citing authors

#	ARTICLE	IF	CITATIONS
1	Revealing the Potential Crystal Structures of Earth-Abundant Nontoxic Photovoltaic CuBi <sub>4</sub> . Crystal Growth and Design, 2021, 21, 2850-2855.	3.0	8
2	Revealing the crystal structures and relative dielectric constants of fluorinated silicon oxides. Journal of Materials Chemistry C, 2021, 9, 15983-15989.	5.5	3
3	Prediction of Fluorooxoborates with Colossal Second Harmonic Generation (SHG) Coefficients and Extremely Wide Band Gaps: Towards Modulating Properties by Tuning the BO <sub>3</sub> /BO <sub>3</sub> F Ratio in Layers. Angewandte Chemie, 2019, 131, 11852-11856.	2.0	16
4	Prediction of Fluorooxoborates with Colossal Second Harmonic Generation (SHG) Coefficients and Extremely Wide Band Gaps: Towards Modulating Properties by Tuning the BO <sub>3</sub> /BO <sub>3</sub> F Ratio in Layers. Angewandte Chemie - International Edition, 2019, 58, 11726-11730.	13.8	66
5	Stable and hard hafnium borides: A first-principles study. Journal of Applied Physics, 2019, 125, .	2.5	13
6	Computer-aided design of metal chalcogenide semiconductors: from chemical composition to crystal structure. Chemical Science, 2018, 9, 1022-1030.	7.4	54
7	New Tungsten Borides, Their Stability and Outstanding Mechanical Properties. Journal of Physical Chemistry Letters, 2018, 9, 3470-3477.	4.6	61
8	Novel high-pressure calcium carbonates. Physical Review B, 2018, 98, .	3.2	32
9	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.	2.8	53
10	Discovering novel VC <sub>1-x</sub> compounds through hybrid first-principles and evolutionary algorithms. Journal of the European Ceramic Society, 2016, 36, 3593-3599.	5.7	10
11	Rational design of inorganic dielectric materials with expected permittivity. Scientific Reports, 2015, 5, 16769.	3.3	14
12	High-pressure structure prediction of Hf-C system and first-principle simulation of their electronic properties. Wuli Xuebao/Acta Physica Sinica, 2015, 64, 236102.	0.5	4
13	Discovering low-permittivity materials: Evolutionary search for MgAl <sub>2</sub> O <sub>4</sub> polymorphs. Applied Physics Letters, 2014, 105, .	3.3	4
14	Evolutionary search for new high- $\kappa$ dielectric materials: methodology and applications to hafnia-based oxides. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 76-84.	0.5	44
15	Monte Carlo simulation of polycrystalline microstructures and finite element stress analysis. Materials & Design, 2014, 55, 740-746.	5.1	18
16	First-principles calculations of the dielectric and vibrational properties of ferroelectric and paraelectric BaAl <sub>2</sub> O <sub>4</sub> . Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 1867-1870.	2.1	15
17	Stressed oxidation life predication of 3D C/SiC composites in a combustion wind tunnel. Composites Science and Technology, 2013, 88, 178-183.	7.8	13
18	Prediction of stable hafnium carbides: Stoichiometries, mechanical properties, and electronic structure. Physical Review B, 2013, 88, .	3.2	51