Chol-Jun Yu

List of Publications by Year
in descending order

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Version: 2024-02-01

60 papers	1,347 citations	393982 19 h-index	377514 34 g-index
61 all docs	61 docs citations	61 times ranked	1903 citing authors

#	Article	IF	Citations
1	First-principles study of ethylene carbonate adsorption on prismatic hard carbon surface: An insight into solid-electrolyte interphase formation. Applied Surface Science, 2022, 573, 151495.	3.1	7
2	Superior thermoelectric properties of ternary chalcogenides CsAg₅Q₃ (Q =) Tj ETQq0 0 0 rgBT /Overlock 10 T 5729-5737.	1.3	4
3	Twofold rattling mode-induced ultralow thermal conductivity in vacancy-ordered double perovskite Cs₂SnI₆. Chemical Communications, 2022, 58, 4223-4226.	2.2	10
4	First-principles study on the elastic, electronic and optical properties of all-inorganic halide perovskite solid solutions of CsPb(Br_{1â^'x}Cl_x)₃ within the virtual crystal approximation. RSC Advances, 2022, 12, 9755-9762.	1.7	2
5	Ab Initio Thermodynamic Study of PbI₂ and CH₃NH₃PbI₃ Surfaces in Reaction with CH₃NH₂ Gas for Perovskite Solar Cells. Journal of Physical Chemistry C, 2022, 126, 3671-3680.	1.5	1
6	Enhancing the Photocatalytic Hydrogen Evolution Performance of the CsPbI₃/MoS₂ Heterostructure with Interfacial Defect Engineering. Journal of Physical Chemistry Letters, 2022, 13, 4007-4014.	2.1	9
7	First-principles study on structural, electronic, magnetic and thermodynamic properties of lithium ferrite LiFe₅O₈. RSC Advances, 2022, 12, 15973-15979.	1.7	2
8	Improving the stability of hybrid perovskite FAPbI₃ by forming 3D/2D interfaces with organic spacers. Chemical Communications, 2022, 58, 8440-8443.	2.2	3
9	First-principles study on structural, electronic and optical properties of perovskite solid solutions KB_{1â^'x}Mg_xI₃ (B = Ge, Sn) toward water splitting photocatalysis. RSC Advances, 2021, 11, 26432-26443.	1.7	11
10	First-principles study of the structural and electrochemical properties of Na_xTi₂O₄ (0 â‰ x â‰ 1) with tunnel structure for anode applications in alkali-ion batteries. Physical Chemistry Chemical Physics, 2021, 23, 8456-8465.	1.3	1
11	High Thermoelectric Performance in the Cubic Inorganic Cesium Iodide Perovskites CsBI₃ (B = Pb, Sn, and Ge) from First-Principles. Journal of Physical Chemistry C, 2021, 125, 6013-6019.	1.5	18
12	Contrary Effect of B and N Doping into Graphene and Graphene Oxide Heterostructures with MoS₂ on Interface Function and Hydrogen Evolution. Journal of Physical Chemistry C, 2021, 125, 6611-6618.	1.5	5
13	Preparation and flame retardant properties of cotton fabrics treated with resorcinol bis(diphenyl) Tj ETQq1 1 0.784314 rgBT /Overlock	2.4	10
14	Interfacial Enhancement of Photovoltaic Performance in MAPbI₃/CsPbI₃ Superlattice. ACS Applied Materials & Interfaces, 2021, 13, 14679-14687.	4.0	13
15	Influence of Metal-Ion Replacement on the Phase Stabilization of Cubic All-Inorganic Cesium Lead Halide Perovskites: an Ab Initio Thermodynamic Formalism for Solution-Processed Cation Doping. Journal of Physical Chemistry C, 2021, 125, 13195-13211.	1.5	9
16	Performance Improvement of Hole-Transport Material-Free Mesoporous Perovskite Solar Cells with Carbon Electrodes Using a Solidâ€“Gas Reaction. ACS Applied Energy Materials, 2021, 4, 6606-6615.	2.5	5
17	Structural and electrochemical trends in mixed manganese oxides <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e610" altimg="si150.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>(M0.44Mn0.56)O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e624" altimg="si187.svg"><mml:msub><mml:mrow	4.0	10
18	Effect of vacancy concentration on the lattice thermal conductivity of CH₃NH₃PbI₃: a molecular dynamics study. RSC Advances, 2021, 11, 34015-34023.	1.7	3

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19	Metal phosphide CuP₂ as a promising thermoelectric material: an insight from a first-principles study. New Journal of Chemistry, 2021, 45, 21569-21576.	1.4	7
20	Computational prediction of structural, electronic, and optical properties and phase stability of double perovskites K₂SnX₆ (X = I, Br, Cl). RSC Advances, 2020, 10, 201-209.	1.7	69
21	Interface Engineering in Hybrid Iodide CH3NH3PbI3 Perovskites Using Lewis Base and Graphene toward High-Performance Solar Cells. ACS Applied Materials & Interfaces, 2020, 12, 1858-1866.	4.0	25
22	First-principles study of luminescence properties of the Eu-doped defect pyrochlore oxide <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>KNbWO</mml:mi><mml:mn>6</mml:mn><mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mo>:</mml:mo><mml:mn>0.125</mml:mn><mml:msup><mml:mrow><mml:mi>Eu</mml:mi> Physical Review B, 2020, 102, .	1.1	3
23	Influence of Ti/V Cation-Exchange in Na₂Ti₃O₇ on Na-Ion Negative Electrode Performance: An Insight from First-Principles Study. Journal of Physical Chemistry C, 2020, 124, 17897-17906.	1.5	11
24	Influence of M/A substitution on material properties of intermetallic compounds MSn2 (M = Fe, and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	1.4	4
25	First-principles study on material properties and stability of inorganic halide perovskite solid solutions CsPb(I1â^'xBrx)3. Physical Review Materials, 2020, 4, .	0.9	10
26	Manifestation of the thermoelectric properties in Ge-based halide perovskites. Physical Review Materials, 2020, 4, .	0.9	14
27	Advances in modelling and simulation of halide perovskites for solar cell applications. JPhys Energy, 2019, 1, 022001.	2.3	53
28	The maximum interbubble distance in relation to the radius of spherical stable nanobubble in liquid water: A molecular dynamics study. Fluid Phase Equilibria, 2019, 487, 45-51.	1.4	9
29	Anharmonic phonons and phase transitions in the vacancy-ordered double perovskite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Cs</mml:mi><mml:mn>2</mml:mn><mml:mi from first-principles predictions. Physical Review B, 2019, 99, .	1.1	38
30	Revealing the Mechanism of Graphene Oxide Reduction by Supercritical Ethanol with First-Principles Calculations. Journal of Physical Chemistry C, 2019, 123, 8932-8942.	1.5	5
31	Vacancy-Driven Stabilization of the Cubic Perovskite Polymorph of CsPbI₃. Journal of Physical Chemistry C, 2019, 123, 9735-9744.	1.5	47
32	Formation and characterization of ceramic coating from alumino silicate mineral powders in the matrix of cement composite on the concrete wall. Materials Chemistry and Physics, 2019, 227, 211-218.	2.0	7
33	First-Principles Study on Structural, Electronic, and Optical Properties of Inorganic Ge-Based Halide Perovskites. Inorganic Chemistry, 2019, 58, 4134-4140.	1.9	68
34	First-principles study of Na_xTiO₂ with trigonal bipyramid structures: an insight into sodium-ion battery anode applications. Physical Chemistry Chemical Physics, 2019, 21, 8408-8417.	1.3	10
35	Defect properties in Yb³⁺-doped CaF₂ from first-principles calculations: a route to defect engineering for up- and down-conversion photoluminescence. Journal of Materials Chemistry C, 2019, 7, 15148-15152.	2.7	8
36	Two-Dimensional Hybrid Composites of SnS₂ with Graphene and Graphene Oxide for Improving Sodium Storage: A First-Principles Study. Inorganic Chemistry, 2019, 58, 1433-1441.	1.9	17

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37	Critical Role of Water in Defect Aggregation and Chemical Degradation of Perovskite Solar Cells. Journal of Physical Chemistry Letters, 2018, 9, 2196-2201.	2.1	104
38	Ab initio design of drug carriers for zoledronate guest molecule using phosphonated and sulfonated calix[4]arene and calix[4]resorcinarene host molecules. Journal of Materials Science, 2018, 53, 5125-5139.	1.7	14
39	Ab initio Investigation of Adsorption Characteristics of Bisphosphonates on Hydroxyapatite (001) Surface. Journal of Materials Science, 2018, 53, 4252-4261.	1.7	42
40	First-principles study of mixed eldfellite compounds <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif"		

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55	Ab initio thermodynamic study of the SnO₂(110) surface in an O₂ and NO environment: a fundamental understanding of the gas sensing mechanism for NO and NO₂. Physical Chemistry Chemical Physics, 2016, 18, 31566-31578.	1.3	22
56	Ab initio investigation of the adsorption of zoledronic acid molecule on hydroxyapatite (001) surface: an atomistic insight of bone protection. Journal of Materials Science, 2016, 51, 3125-3135.	1.7	13
57	Refined phase coexistence line between graphite and diamond from density-functional theory and van der Waals correction. Physica B: Condensed Matter, 2014, 434, 185-193.	1.3	20
58	Ab initio modeling of glass corrosion: Hydroxylation and chemisorption of oxalic acid at diopside and Ã¥kermanite surfaces. Acta Materialia, 2009, 57, 5303-5313.	3.8	6
59	An efficient virtual crystal approximation that can be used to treat heterovalent atoms, applied to (1â^'x)BiScO₃â€“xPbTiO₃. Journal of Physics Condensed Matter, 2007, 19, 306203.	0.7	28
60	Characterization of compositional particles in eye shadow powder by scanning electron microscope and Xâ€ray mapping. X-Ray Spectrometry, 0, , .	0.9	0