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	Influence of halide composition on the structural, electronic, and optical properties of mixed<mml:math		

#	Article	IF	Citations
19	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
20	Revealing the formation and electrochemical properties of bis(trifluoromethanesulfonyl)imide intercalated graphite with first-principles calculations. Physical Chemistry Chemical Physics, 2018, 20, 14124-14132.	1.3	19
21	Electronic structure and photoabsorption property of pseudocubic perovskites CH3NH3PbX3(XÂ=ÂI, Br) including van der Waals interaction. Journal of Materials Science, 2016, 51, 9849-9854.	1.7	18
22	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
23	First-principles study of ferroelectricity induced by pâ€“d hybridization in ferrimagnetic NiFe 2 O 4. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 3302-3306.	0.9	17
24	Ionic Diffusion and Electronic Transport in Eldfellite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Na</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:mi>Fe</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:msub><mml:mi>SO</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:msub><mml:mo	1.5	17
25	2017, 8, . 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
26	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
27	Manifestation of the thermoelectric properties in Ge-based halide perovskites. Physical Review Materials, 2020, 4, .	0.9	14
28	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
29	Interfacial Enhancement of Photovoltaic Performance in MAPbI₃/CsPbI₃ Superlattice. ACS Applied Materials & Interfaces, 2021, 13, 14679-14687.	4.0	13
30	First-principles study of mixed eldfellite compounds <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif"		

#	Article	IF	Citations
37	Twofold rattling mode-induced ultralow thermal conductivity in vacancy-ordered double perovskite Cs₂SnI₆. Chemical Communications, 2022, 58, 4223-4226.	2.2	10
38	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
39	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
40	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
41	First-principles study of organically modifiedÂmuscovite mica with ammonium (NH $$_4^+$$ 4 +) or methylammonium (CH $$_3$$ 3 NH $$_3^+$$ 3 +) ion. Journal of Materials Science, 2016, 51, 10806-10818.	1.7	8
42	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
43	Mechanism of ultraviolet upconversion luminescence of Gd3+ ions sensitized by Yb3+-clusters in CaF2:Yb3+, Gd3+. Journal of Luminescence, 2018, 194, 72-74.	1.5	7
44	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
45	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
46	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
47	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
48	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
49	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
50	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
51	Influence of M/A substitution on material properties of intermetallic compounds MSn2 (M = Fe, and) Tj ETQq1 1 0.784314 rgBT /Over	1.4	4
52	Superior thermoelectric properties of ternary chalcogenides CsAg₅Q₃ (Q =) Tj ETQq0 0 0 rgBT /Overlock 10 T 5729-5737.	1.3	4
53	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
54	Effect of vacancy concentration on the lattice thermal conductivity of CH₃NH₃PbI₃: a molecular dynamics study. RSC Advances, 2021, 11, 34015-34023.	1.7	3

#	Article	IF	Citations
55	Improving the stability of hybrid perovskite FAPbI₃ by forming 3D/2D interfaces with organic spacers. Chemical Communications, 2022, 58, 8440-8443.	2.2	3
56	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
57	First-principles study on structural, electronic, magnetic and thermodynamic properties of lithium ferrite LiFe₅O₈. RSC Advances, 2022, 12, 15973-15979.	1.7	2
58	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
59	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
60	Characterization of compositional particles in eye shadow powder by scanning electron microscope and Xâ€ray mapping. X-Ray Spectrometry, 0, , .	0.9	0