Guocai Tian

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9594521/publications.pdf

Version: 2024-02-01

48	406	933264	839398
papers	citations	10	18
		h-index	g-index

49	49	49	436
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	First-principles calculations to investigate Zr substitution enhanced thermoelectric performance of p-type Zr Hf1â^'CoBi (xâ€ =â€0,0.25,0.5,0.75,1) compounds. Physics Letters, Section A: General, Atomic and Solid State Physics, 2022, 424, 127839.	2.9	2
2	First-principles studies of imidazolium chloroaluminate ionic liquids with different substitutions on the Pt(111) surface. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 635, 128079.	2.3	1
3	First-principle investigation on the thermoelectric properties of XCoGe (X = V, Nb, and Ta) half-Heusler compounds. Materials Science in Semiconductor Processing, 2022, 140, 106387.	1.9	9
4	Computational prediction of high thermoelectric performance in MPtSn (M = Ti, Zr, and Hf) half-Heusler compounds by first-principle study. Solid State Sciences, 2022, 127, 106859.	1.5	5
5	First-principle investigation on the thermoelectric and electronic properties of HfCoX (X=As, Sb, Bi) half-Heusler compounds. Journal of Solid State Chemistry, 2022, 314, 123386.	1.4	8
6	Research on the mechanism of synergistic-dehydration/detoxification for sludge under treatment with double-modified potato residue. Chemical Engineering Journal, 2021, 420, 127699.	6.6	4
7	Effects of flocculant-modified phosphogypsum on sludge treatment: investigation of the operating parameters, variations of the chemical groups, and heavy metals in the sludge. Environmental Science: Water Research and Technology, 2021, 7, 184-196.	1.2	0
8	First Principle Analysis on Pyridine Amide Derivativesâ€™ Adsorption Behavior on the Pt (111) Surface. Crystals, 2021, 11, 98.	1.0	2
9	Applications of green solvents in toxic gases removal. , 2021, , 149-201.		4
10	Characterization of the Interface Structure of 1-Ethyl-2,3-alkylimidazolium Bis(trifluoromethylsulfonyl)imide on a Au(111) Surface with Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2021, 125, 3677-3689.	1.2	8
11	Structural Characterization and Molecular Simulation of Baoqing Lignite. ACS Omega, 2021, 6, 10281-10287.	1.6	3
12	Adsorption and inhibition behavior of imidazolium tetrafluoroborate derivatives as green corrosion inhibitors for carbon steel. Journal of Molecular Modeling, 2021, 27, 195.	0.8	11
13	Theoretical prediction of transport coefficients of antimony doped tin dioxide. Ceramics International, 2021, 47, 15277-15281.	2.3	4
14	Develop a green sludge treatment: Effects of a new additive on sludge properties and co-removal of bound water, organics and toxic elements in sludge. Journal of Cleaner Production, 2021, 304, 127148.	4.6	4
15	Performance and Mechanism of Alkylimidazolium Ionic Liquids as Corrosion Inhibitors for Copper in Sulfuric Acid Solution. Molecules, 2021, 26, 4910.	1.7	8
16	Effect of acetonitrile on the interface structure of Au (1 0 0)/1-butyl-3-methyl tetrafluoroborate ionic liquid determined by a molecular dynamics simulation. Chemical Physics Letters, 2021, 779, 138882.	1.2	0
17	High thermoelectric performance of half-Heusler ZrXPb (X = Ni, Pd, and Pt) compounds from first principle calculation. Journal of Physics Condensed Matter, 2021, 33, 465501.	0.7	6
18	Extraction of copper from chalcopyrite with potassium dichromate in 1-ethyl-3-methylimidazolium hydrogen sulfate ionic liquid aqueous solution. Minerals Engineering, 2021, 172, 107179.	1.8	5

#	Article	IF	Citations
19	The Influence of Anion Structure on the Ionic Liquids/Au (100) Interface by Molecular Dynamics Simulations. Langmuir, 2021, 37, 14059-14071.	1.6	12
20	The Effects of Benzene on the Structure and Properties of Triethylamine Hydrochloride/Chloroaluminate. Crystals, 2021, 11, 1532.	1.0	0
21	Combining theory and experiment to determine thermoelectrics of tellurium doped CoSb3. Intermetallics, 2020, 125, 106918.	1.8	5
22	Effect of Aluminium Fluoride on the Structure and Properties of Cryolite Alumina Molten Salt System. Journal of Physics: Conference Series, 2020, 1637, 012093.	0.3	0
23	Electrical Double-Layer Structure and Property of Ionic Liquid-Electrode System for Electrochemical Applications. Nanotechnology in the Life Sciences, 2020, , 177-220.	0.4	0
24	Accurate excitation energies of molecules and oligomers from a semilocal density functional. Journal of Chemical Physics, 2017, 146, 234102.	1.2	11
25	Comparative study of semilocal density functionals on solids and surfaces. Chemical Physics Letters, 2017, 682, 38-42.	1.2	12
26	Leaching of chalcopyrite with hydrogen peroxide in 1-hexyl-3-methyl-imidazolium hydrogen sulfate ionic liquid aqueous solution. Hydrometallurgy, 2017, 169, 1-8.	1.8	30
27	Performance of a nonempirical exchange functional from density matrix expansion: comparative study with different correlations. Physical Chemistry Chemical Physics, 2017, 19, 21707-21713.	1.3	20
28	Effects of Molecular Structure and Solvent Polarity on Adsorption of Carboxylic Anchoring Dyes onto TiO₂ Particles in Aprotic Solvents. Langmuir, 2017, 33, 7036-7042.	1.6	19
29	Energetic Study of Clusters and Reaction Barrier Heights from Efficient Semilocal Density Functionals. Computation, 2017, 5, 27.	1.0	7
30	Performance of a nonempirical density functional on molecules and hydrogen-bonded complexes. Journal of Chemical Physics, 2016, 145, 234306.	1.2	25
31	Accurate van der Waals coefficients between fullerenes and fullerene-alkali atoms and clusters: Modified single-frequency approximation. Physical Review B, 2016, 94, .	1.1	12
32	Molecular Dynamics Simulation of Effects of NH₄Cl on the Properties of Lewis Acidic 1-Ethyl-3-Methyl-Imidazolium Chloride/Chloroaluminate Molten Salts. Advanced Materials Research, 2013, 791-793, 183-186.	0.3	0
33	Simulation of the Structure and Properties of Room Temperature Molten Salts 1-Ethyl-3-Methyl-Imidazolium Chloride/Chloroaluminate. Advanced Materials Research, 2012, 430-432, 547-550.	0.3	2
34	Simulation of the Properties of 1-Ethyl-3-Methyl-Imidazolium Chloride/Chloroaluminate Ionic Liquids: Concentration and Temperature Dependence. Advanced Materials Research, 2012, 457-458, 249-252.	0.3	2
35	Application of Ionic Liquids in Extraction and Separation of Metals. , 2012, , 119-153.		5
36	Study on the Structure and Spectrum of Water in 1-Ethyl-3-Methylimidazolium Tetrafluoroborate Ionic Liquids. Advanced Materials Research, 2011, 271-273, 92-97.	0.3	0

#	Article	IF	Citations
37	MOLECULAR DYNAMICS SIMULATION ON THE STRUCTURE AND DYNAMICS OF WATER IN THE 1-BUTYL-3-METHYLIMIDAZOLIUM TETRAFLUOROBORATE/WATER MIXTURE. Journal of Theoretical and Computational Chemistry, 2010, 09, 573-584.	1.8	4
38	Application of ionic liquids in hydrometallurgy of nonferrous metals. Transactions of Nonferrous Metals Society of China, 2010, 20, 513-520.	1.7	109
39	Computer simulation study on the structure and spectrum of water in BF<inf>4</inf>[−] solvation shell. , 2009, , .		0
40	Simulation Study on the Structure and Dynamics of Water in Sodium Tetrafluoroborate/Water. Chinese Journal of Chemical Physics, 2009, 22, 460-466.	0.6	7
41	Quantum chemical aided molecular design of ionic liquids as green electrolytes for electrodeposition of active metals. Transactions of Nonferrous Metals Society of China, 2009, 19, 1639-1644.	1.7	10
42	Numerical Study of Vibrational Energy Relaxation of OH Bending in Liquid H2O. Chinese Journal of Chemical Physics, 2007, 20, 541-546.	0.6	5
43	Molecular dynamics study on the vibrational energy relaxation of Oâ€“D stretch of HOD in liquid H2O. Chemical Physics, 2006, 328, 216-220.	0.9	9
44	Study of Relations between Position and Momentum Expectation Values for Molecules. Physica Scripta, 2002, 66, 449-453.	1.2	3
45	Study of Effect of Water on the Physicochemical Properties of 1-Buthyl-3-Methylimidazolium Chloride Ionic Liquids. Advanced Materials Research, 0, 549, 152-156.	0.3	9
46	Study on the Physicochemical Properties of the Mixture of Water and 1-butyl-3-methylimidazolium Hydrogen Sulfate Salt Ionic Liquids. Advanced Materials Research, 0, 887-888, 643-646.	0.3	1
47	Simulation of the Properties of 1-Ethyl-3-Methyl-Imidazolium Chloride/Chloroaluminate Ionic Liquids: Concentration and Temperature Dependence. Advanced Materials Research, 0, 457-458, 249-252.	0.3	0
48	Lanthanum-doped SrTiO3 theoretical thermoelectric properties. Ionics, 0, , 1.	1.2	3