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	932766 10	839053 18
papers	citations	h-index	g-index

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

#	Article	IF	Citations
1	Application of ionic liquids in hydrometallurgy of nonferrous metals. Transactions of Nonferrous Metals Society of China, 2010, 20, 513-520.	1.7	109
2	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
3	Performance of a nonempirical density functional on molecules and hydrogen-bonded complexes. Journal of Chemical Physics, 2016, 145, 234306.	1.2	25
4	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
5	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
6	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
7	Comparative study of semilocal density functionals on solids and surfaces. Chemical Physics Letters, 2017, 682, 38-42.	1.2	12
8	The Influence of Anion Structure on the Ionic Liquids/Au (100) Interface by Molecular Dynamics Simulations. Langmuir, 2021, 37, 14059-14071.	1.6	12
9	Accurate excitation energies of molecules and oligomers from a semilocal density functional. Journal of Chemical Physics, 2017, 146, 234102.	1.2	11
10	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
11	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
12	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
13	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
14	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
15	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
16	Performance and Mechanism of Alkylimidazolium Ionic Liquids as Corrosion Inhibitors for Copper in Sulfuric Acid Solution. Molecules, 2021, 26, 4910.	1.7	8
17	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
18	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

#	Article	IF	Citations
19	Energetic Study of Clusters and Reaction Barrier Heights from Efficient Semilocal Density Functionals. Computation, 2017, 5, 27.	1.0	7
20	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
21	Numerical Study of Vibrational Energy Relaxation of OH Bending in Liquid H2O. Chinese Journal of Chemical Physics, 2007, 20, 541-546.	0.6	5
22	Application of Ionic Liquids in Extraction and Separation of Metals. , 2012, , 119-153.		5
23	Combining theory and experiment to determine thermoelectrics of tellurium doped CoSb3. Intermetallics, 2020, 125, 106918.	1.8	5
24	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
25	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
26	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
27	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
28	Applications of green solvents in toxic gases removal. , 2021, , 149-201.		4
29	Theoretical prediction of transport coefficients of antimony doped tin dioxide. Ceramics International, 2021, 47, 15277-15281.	2.3	4
30	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
31	Study of Relations between Position and Momentum Expectation Values for Molecules. Physica Scripta, 2002, 66, 449-453.	1.2	3
32	Structural Characterization and Molecular Simulation of Baoqing Lignite. ACS Omega, 2021, 6, 10281-10287.	1.6	3
33	Lanthanum-doped SrTiO3 theoretical thermoelectric properties. Ionics, 0, , 1.	1.2	3
34	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
35	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
36	First Principle Analysis on Pyridine Amide Derivativesâ€™ Adsorption Behavior on the Pt (111) Surface. Crystals, 2021, 11, 98.	1.0	2

#	Article	IF	Citations
37	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
38	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
39	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
40	Computer simulation study on the structure and spectrum of water in BF<inf>4</inf>[−] solvation shell. , 2009, , .		0
41	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
42	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
43	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
44	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
45	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
46	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
47	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
48	The Effects of Benzene on the Structure and Properties of Triethylamine Hydrochloride/Chloroaluminate. Crystals, 2021, 11, 1532.	1.0	0