

Guocai Tian

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	First-principles calculations to investigate Zr substitution enhanced thermoelectric performance of p-type Zr Hf _{1-x} CoBi (x = 0, 0.25, 0.5, 0.75, 1) compounds. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2022, 424, 127839.		2
2	First-principles studies of imidazolium chloroaluminate ionic liquids with different substitutions on the Pt(111) surface. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 635, 128079.	4.7	1
3	First-principle investigation on the thermoelectric properties of XCoGe (X = V, Nb, and Ta) half-Heusler compounds. <i>Materials Science in Semiconductor Processing</i> , 2022, 140, 106387.	4.0	9
4	Computational prediction of high thermoelectric performance in MPtSn (M = Ti, Zr, and Hf) half-Heusler compounds by first-principle study. <i>Solid State Sciences</i> , 2022, 127, 106859.	3.2	5
5	First-principle investigation on the thermoelectric and electronic properties of HfCoX (X=As, Sb, Bi) half-Heusler compounds. <i>Journal of Solid State Chemistry</i> , 2022, 314, 123386.	2.9	8
6	Research on the mechanism of synergistic-dehydration/detoxification for sludge under treatment with double-modified potato residue. <i>Chemical Engineering Journal</i> , 2021, 420, 127699.	12.7	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. <i>Environmental Science: Water Research and Technology</i> , 2021, 7, 184-196.	2.4	0
8	First Principle Analysis on Pyridine Amide Derivatives™ Adsorption Behavior on the Pt (111) Surface. <i>Crystals</i> , 2021, 11, 98.	2.2	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. <i>Journal of Physical Chemistry B</i> , 2021, 125, 3677-3689.	2.6	8
11	Structural Characterization and Molecular Simulation of Baoqing Lignite. <i>ACS Omega</i> , 2021, 6, 10281-10287.	3.5	3
12	Adsorption and inhibition behavior of imidazolium tetrafluoroborate derivatives as green corrosion inhibitors for carbon steel. <i>Journal of Molecular Modeling</i> , 2021, 27, 195.	1.8	11
13	Theoretical prediction of transport coefficients of antimony doped tin dioxide. <i>Ceramics International</i> , 2021, 47, 15277-15281.	4.8	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. <i>Journal of Cleaner Production</i> , 2021, 304, 127148.	9.3	4
15	Performance and Mechanism of Alkylimidazolium Ionic Liquids as Corrosion Inhibitors for Copper in Sulfuric Acid Solution. <i>Molecules</i> , 2021, 26, 4910.	3.8	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. <i>Chemical Physics Letters</i> , 2021, 779, 138882.	2.6	0
17	High thermoelectric performance of half-Heusler ZrXPb (X = Ni, Pd, and Pt) compounds from first principle calculation. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 465501.	1.8	6
18	Extraction of copper from chalcopyrite with potassium dichromate in 1-ethyl-3-methylimidazolium hydrogen sulfate ionic liquid aqueous solution. <i>Minerals Engineering</i> , 2021, 172, 107179.	4.3	5

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19	The Influence of Anion Structure on the Ionic Liquids/Au (100) Interface by Molecular Dynamics Simulations. <i>Langmuir</i> , 2021, 37, 14059-14071.	3.5	12
20	The Effects of Benzene on the Structure and Properties of Triethylamine Hydrochloride/Chloroaluminate. <i>Crystals</i> , 2021, 11, 1532.	2.2	0
21	Combining theory and experiment to determine thermoelectrics of tellurium doped CoSb ₃ . <i>Intermetallics</i> , 2020, 125, 106918.	3.9	5
22	Effect of Aluminium Fluoride on the Structure and Properties of Cryolite Alumina Molten Salt System. <i>Journal of Physics: Conference Series</i> , 2020, 1637, 012093.	0.4	0
23	Electrical Double-Layer Structure and Property of Ionic Liquid-Electrode System for Electrochemical Applications. <i>Nanotechnology in the Life Sciences</i> , 2020, , 177-220.	0.6	0
24	Accurate excitation energies of molecules and oligomers from a semilocal density functional. <i>Journal of Chemical Physics</i> , 2017, 146, 234102.	3.0	11
25	Comparative study of semilocal density functionals on solids and surfaces. <i>Chemical Physics Letters</i> , 2017, 682, 38-42.	2.6	12
26	Leaching of chalcopyrite with hydrogen peroxide in 1-hexyl-3-methyl-imidazolium hydrogen sulfate ionic liquid aqueous solution. <i>Hydrometallurgy</i> , 2017, 169, 1-8.	4.3	30
27	Performance of a nonempirical exchange functional from density matrix expansion: comparative study with different correlations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21707-21713.	2.8	20
28	Effects of Molecular Structure and Solvent Polarity on Adsorption of Carboxylic Anchoring Dyes onto TiO ₂ Particles in Aprotic Solvents. <i>Langmuir</i> , 2017, 33, 7036-7042.	3.5	19
29	Energetic Study of Clusters and Reaction Barrier Heights from Efficient Semilocal Density Functionals. <i>Computation</i> , 2017, 5, 27.	2.0	7
30	Performance of a nonempirical density functional on molecules and hydrogen-bonded complexes. <i>Journal of Chemical Physics</i> , 2016, 145, 234306.	3.0	25
31	Accurate van der Waals coefficients between fullerenes and fullerene-alkali atoms and clusters: Modified single-frequency approximation. <i>Physical Review B</i> , 2016, 94, .	3.2	12
32	Molecular Dynamics Simulation of Effects of NH ₄ Cl on the Properties of Lewis Acidic 1-Ethyl-3-Methyl-Imidazolium Chloride/Chloroaluminate Molten Salts. <i>Advanced Materials Research</i> , 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. <i>Advanced Materials Research</i> , 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. <i>Advanced Materials Research</i> , 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. <i>Advanced Materials Research</i> , 2011, 271-273, 92-97.	0.3	0

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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.	4.2	109
39	Computer simulation study on the structure and spectrum of water in BF ₄ ⁻ ; 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.	1.3	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.	4.2	10
42	Numerical Study of Vibrational Energy Relaxation of OH Bending in Liquid H ₂ O. Chinese Journal of Chemical Physics, 2007, 20, 541-546.	1.3	5
43	Molecular dynamics study on the vibrational energy relaxation of O-H stretch of HOD in liquid H ₂ O. Chemical Physics, 2006, 328, 216-220.	1.9	9
44	Study of Relations between Position and Momentum Expectation Values for Molecules. Physica Scripta, 2002, 66, 449-453.	2.5	3
45	Study of Effect of Water on the Physicochemical Properties of 1-Butyl-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 SrTiO ₃ theoretical thermoelectric properties. Ionics, 0, , 1.	2.4	3