

Zijing Lin

List of Publications by Year in descending order

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104
papers

2,716
citations

147801

31
h-index

206112

48
g-index

104
all docs

104
docs citations

104
times ranked

2177
citing authors

#	ARTICLE	IF	CITATIONS
1	Percolation theory to predict effective properties of solid oxide fuel-cell composite electrodes. <i>Journal of Power Sources</i> , 2009, 191, 240-252.	7.8	176
2	Gaseous Arginine Conformers and Their Unique Intramolecular Interactions. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12282-12291.	2.5	100
3	The effects of the interconnect rib contact resistance on the performance of planar solid oxide fuel cell stack and the rib design optimization. <i>Journal of Power Sources</i> , 2008, 183, 214-225.	7.8	90
4	A key geometric parameter for the flow uniformity in planar solid oxide fuel cell stacks. <i>International Journal of Hydrogen Energy</i> , 2009, 34, 3873-3884.	7.1	78
5	Detailed Ab Initio Studies of the Conformers and Conformational Distributions of Gaseous Tryptophan. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2656-2659.	2.5	75
6	A multiphysics fully coupled modeling tool for the design and operation analysis of planar solid oxide fuel cell stacks. <i>Applied Energy</i> , 2017, 190, 1234-1244.	10.1	75
7	Exploration of the full conformational landscapes of gaseous aromatic amino acid phenylalanine: An ab initio study. <i>Computational and Theoretical Chemistry</i> , 2006, 758, 195-202.	1.5	70
8	A modified dusty gas model in the form of a Fick's model for the prediction of multicomponent mass transport in a solid oxide fuel cell anode. <i>Journal of Power Sources</i> , 2012, 206, 171-178.	7.8	70
9	Heat transfer in the dynamic cycling of lithium-titanate batteries. <i>International Journal of Heat and Mass Transfer</i> , 2016, 93, 896-905.	4.8	69
10	The influence of interconnect ribs on the performance of planar solid oxide fuel cell and formulae for optimal rib sizes. <i>Journal of Power Sources</i> , 2012, 204, 106-115.	7.8	67
11	Combined micro-scale and macro-scale modeling of the composite electrode of a solid oxide fuel cell. <i>Journal of Power Sources</i> , 2010, 195, 6598-6610.	7.8	66
12	Systematic ab initio studies of the conformers and conformational distribution of gas-phase tyrosine. <i>Journal of Chemical Physics</i> , 2005, 122, 134313.	3.0	62
13	Three-dimensional modeling of planar solid oxide fuel cells and the rib design optimization. <i>Journal of Power Sources</i> , 2009, 194, 854-863.	7.8	62
14	The effect of interconnect rib size on the fuel cell concentration polarization in planar SOFCs. <i>Journal of Power Sources</i> , 2003, 117, 92-97.	7.8	61
15	Protonation Processes and Electronic Spectra of Histidine and Related Ions. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4340-4352.	2.5	61
16	Comparison of some representative density functional theory and wave function theory methods for the studies of amino acids. <i>Journal of Computational Chemistry</i> , 2009, 30, 589-600.	3.3	61
17	Spin current generation by adiabatic pumping in monolayer graphene. <i>Applied Physics Letters</i> , 2011, 98, .	3.3	59
18	Continuum scale modelling and complementary experimentation of solid oxide cells. <i>Progress in Energy and Combustion Science</i> , 2021, 85, 100902.	31.2	58

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19	Numerical study on the mechanical stress and mechanical failure of planar solid oxide fuel cell. <i>Applied Energy</i> , 2018, 229, 63-68.	10.1	49
20	Effects of Electrode Composition and Thickness on the Mechanical Performance of a Solid Oxide Fuel Cell. <i>Energies</i> , 2018, 11, 1735.	3.1	47
21	Adsorption and properties of aromatic amino acids on single-walled carbon nanotubes. <i>Nanoscale</i> , 2012, 4, 1146-1153.	5.6	45
22	Ab initio studies of aspartic acid conformers in gas phase and in solution. <i>Journal of Chemical Physics</i> , 2007, 127, 154314.	3.0	44
23	Effects of electrode composition on the electrochemical performance and mechanical property of micro-tubular solid oxide fuel cell. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 12925-12940.	7.1	44
24	Quantum pumping of valley current in strain engineered graphene. <i>Applied Physics Letters</i> , 2014, 104, .	3.3	42
25	Coexistence of Dihydrogen, Blue- and Red-Shifting Hydrogen Bonds in an Ultrasmall System: Valine. <i>ChemPhysChem</i> , 2006, 7, 828-830.	2.1	40
26	Degradations of the electrochemical performance of solid oxide fuel cell induced by material microstructure evolutions. <i>Applied Energy</i> , 2018, 231, 22-28.	10.1	40
27	A semi-empirical and ab initio combined approach for the full conformational searches of gaseous lysine and lysine-H ₂ O complex. <i>Computational and Theoretical Chemistry</i> , 2008, 858, 52-65.	1.5	39
28	LDA and GGA calculations of alkali metal adsorption at the (001) surface of MgO. <i>Journal of Chemical Physics</i> , 2000, 112, 3014-3022.	3.0	38
29	A theoretical framework for multiphysics modeling of methane fueled solid oxide fuel cell and analysis of low steam methane reforming kinetics. <i>Applied Energy</i> , 2016, 176, 1-11.	10.1	37
30	First-principle studies of gaseous aromatic amino acid histidine. <i>Computational and Theoretical Chemistry</i> , 2006, 801, 7-20.	1.5	35
31	Theoretical studies on the electrochemical and mechanical properties and microstructure optimization of micro-tubular solid oxide fuel cells. <i>Journal of Power Sources</i> , 2013, 232, 106-122.	7.8	34
32	Ab initio studies of gas phase asparagine conformers. <i>Computational and Theoretical Chemistry</i> , 2005, 719, 153-158.	1.5	32
33	Extensive conformational searches of 13 representative dipeptides and an efficient method for dipeptide structure determinations based on amino acid conformers. <i>Journal of Computational Chemistry</i> , 2009, 30, 2105-2121.	3.3	32
34	Theoretical model for surface diffusion driven Ni-particle agglomeration in anode of solid oxide fuel cell. <i>Journal of Power Sources</i> , 2014, 255, 144-150.	7.8	29
35	Flow uniformity optimization for large size planar solid oxide fuel cells with U-type parallel channel designs. <i>Journal of Power Sources</i> , 2010, 195, 3207-3214.	7.8	28
36	Ab initio studies of the conformers and conformational distribution of the gaseous hydroxyamino acid threonine. <i>Computational and Theoretical Chemistry</i> , 2006, 760, 159-166.	1.5	27

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37	Effects of microsolvation and aqueous solvation on the tautomers of histidine: a computational study on energy, structure and IR spectrum. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 37-47.	1.4	27
38	Exploration of tetrahedral structures in silicate cathodes using a motif-network scheme. <i>Scientific Reports</i> , 2015, 5, 15555.	3.3	27
39	Parametric study of kW-class solid oxide fuel cell stacks fueled by hydrogen and methane with fully multiphysical coupling model. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 9488-9502.	7.1	26
40	Comprehensive computational study of gas-phase conformations of neutral, protonated and deprotonated glutamic acids. <i>Computational and Theoretical Chemistry</i> , 2011, 976, 42-50.	2.5	23
41	First-Principles Study on Core-Level Spectroscopy of Arginine in Gas and Solid Phases. <i>Journal of Physical Chemistry B</i> , 2012, 116, 12641-12650.	2.6	23
42	A Microscale Modeling Tool for the Design and Optimization of Solid Oxide Fuel Cells. <i>Energies</i> , 2009, 2, 427-444.	3.1	22
43	An exploration of conformational search of leucine molecule and their vibrational spectra in gas phase using ab initio methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009, 73, 865-870.	3.9	22
44	Structural stabilities of metalated histidines in gas phase and existence of gaseous zwitterionic histidine conformers. <i>Computational and Theoretical Chemistry</i> , 2009, 895, 65-71.	1.5	20
45	Comprehensive ab initio study on the conformations of L-Threonine and L-allo-Threonine and related species in gas phase. <i>Computational and Theoretical Chemistry</i> , 2010, 962, 23-32.	1.5	19
46	Conformational search for zwitterionic leucine and hydrated conformers of both the canonical and zwitterionic leucine using the DFT-CPCM model. <i>Vibrational Spectroscopy</i> , 2011, 56, 74-81.	2.2	19
47	A Schottky barrier based model for the grain size effect on oxygen ion conductivity of acceptor-doped ZrO ₂ and CeO ₂ . <i>International Journal of Hydrogen Energy</i> , 2014, 39, 14334-14341.	7.1	19
48	Adsorption of CO on MgO supported alkali monolayers: a periodic density functional local density approximation and generalized gradient approximation study. <i>Surface Science</i> , 2000, 445, 495-505.	1.9	18
49	Spin polarization switching in monolayer graphene through a Rashba multi-barrier structure. <i>Applied Physics Letters</i> , 2013, 102, .	3.3	18
50	Gas-phase IR spectroscopy of deprotonated amino acids: Global or Local minima?. <i>Chemical Physics Letters</i> , 2014, 598, 86-90.	2.6	18
51	Comprehensive Conformational Studies of Five Tripeptides and a Deduced Method for Efficient Determinations of Peptide Structures. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2269-2283.	2.6	17
52	Pure valley current generation in graphene with a Dirac gap by quantum pumping. <i>Applied Physics Express</i> , 2014, 7, 125102.	2.4	17
53	Multicenter Integration Scheme for Electronic Structure Calculations of Periodic and Nonperiodic Polyatomic Systems. <i>Journal of Physical Chemistry A</i> , 1999, 103, 2117-2127.	2.5	16
54	Long-term evolution of mechanical performance of solid oxide fuel cell stack and the underlying mechanism. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 24293-24304.	7.1	16

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55	Comprehensive Density Functional Theory Study on the Mechanism of Activation of the Nonapeptide Hormone Oxytocin by Metal Ions. <i>Journal of Physical Chemistry B</i> , 2010, 114, 1417-1423.	2.6	14
56	Atomic nitrogen chemisorption on graphene with extended line defects. <i>Journal of Materials Chemistry</i> , 2012, 22, 21167.	6.7	14
57	Spin transport in graphene spin-orbit barrier structure. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2013, 377, 632-636.	2.1	13
58	A fragment based step-by-step strategy for determining the most stable conformers of biomolecules. <i>Chemical Physics Letters</i> , 2014, 610-611, 303-309.	2.6	13
59	Fe-Si networks and charge/discharge-induced phase transitions in $\text{Li}_{2\text{FeSiO}_4}$ cathode materials. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 14557-14563.	2.8	12
60	Thorough theoretical search of conformations of neutral, protonated and deprotonated glutamine in gas phase. <i>Computational and Theoretical Chemistry</i> , 2013, 1020, 14-21.	2.5	11
61	Point defect weakened thermal contraction in monolayer graphene. <i>Journal of Chemical Physics</i> , 2014, 141, 064705.	3.0	11
62	Effects of methane steam reforming on the mechanical stability of solid oxide fuel cell stack. <i>Applied Energy</i> , 2022, 322, 119464.	10.1	11
63	Extensive Computational Study on Coordination of Transition Metal Cations and Water Molecules to Glutamic Acid. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7177-7188.	2.5	10
64	Zwitterions are the most stable form for neutral arginylglycine in gas phase: Clear theoretical evidence. <i>Computational and Theoretical Chemistry</i> , 2013, 1008, 96-102.	2.5	9
65	Theoretical models for effective electrical and electrochemical properties of nano-particle infiltrated electrode of solid oxide fuel cell. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 15982-15988.	7.1	9
66	Complexations of alkali/alkaline earth metal cations with gaseous glutamic acid. <i>Computational and Theoretical Chemistry</i> , 2014, 1039, 1-10.	2.5	9
67	A genetic algorithm encoded with the structural information of amino acids and dipeptides for efficient conformational searches of oligopeptides. <i>Journal of Computational Chemistry</i> , 2016, 37, 1214-1222.	3.3	9
68	A scheme for the generation of Fe-P networks to search for low-energy LiFePO_4 crystal structures. <i>Journal of Materials Chemistry A</i> , 2017, 5, 14611-14618.	10.3	9
69	Optimization Design of Rib Width and Performance Analysis of Solid Oxide Electrolysis Cell. <i>Energies</i> , 2020, 13, 5468.	3.1	9
70	Generation of large spin currents in graphene using adiabatic quantum pumping. <i>Journal of Applied Physics</i> , 2012, 112, 073701.	2.5	8
71	Property models and theoretical analysis of novel solid oxide fuel cell with triplet nano-composite electrode. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 13763-13769.	7.1	8
72	Stabilizing the crystal structures of NaFePO_4 with Li substitutions. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 13975-13980.	2.8	8

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73	Theoretical search for possible Li-Ni-B crystal structures using an adaptive genetic algorithm. Journal of Applied Physics, 2020, 127, .	2.5	8
74	Elementary reaction pathway study and a deduced macrokinetic model for the unified understanding of Ni-catalyzed steam methane reforming. Reaction Chemistry and Engineering, 2020, 5, 873-885.	3.7	8
75	A COMPARATIVE STUDY ON INTERMOLECULAR HYDROGEN BOND INTERACTIONS IN MOLECULAR DIMERS USING DIFFERENT LEVELS OF COMPUTATIONAL METHODS. Journal of Theoretical and Computational Chemistry, 2012, 11, 1237-1259.	1.8	7
76	Inducing extended line defects in graphene by linear adsorption of C and N atoms. Applied Physics Letters, 2012, 101, .	3.3	7
77	The role of dimerization on the structure transformation of arginine in gas phase. Chemical Physics Letters, 2014, 608, 398-403.	2.6	7
78	Theoretical spectroscopic studies on chemical and electronic structures of arginylglycine. Physical Chemistry Chemical Physics, 2015, 17, 24754-24760.	2.8	7
79	Pulay forces in density functional theory for periodic and molecular systems. Physics Letters, Section A: General, Atomic and Solid State Physics, 2002, 299, 413-417.	2.1	6
80	Ternary Zinc Antimonides Unlocked Using Hydride Synthesis. Inorganic Chemistry, 2021, 60, 10686-10697.	4.0	6
81	Density Functional Theory Based Micro- and Macro-Kinetic Studies of Ni-Catalyzed Methanol Steam Reforming. Catalysts, 2020, 10, 349.	3.5	5
82	A Simple Scheme for Studies of Surface Phonons of Covalent Semiconductors. I. Calculation of Force Constants. Physica Status Solidi (B): Basic Research, 1988, 148, 525-532.	1.5	4
83	A Simple Scheme for Studies of Surface Phonons of Covalent Semiconductors. II. Surface Phonons at Ideal and Relaxed Si(110) Surface. Physica Status Solidi (B): Basic Research, 1988, 149, 143-148.	1.5	4
84	Transverse currents in triplet Josephson junction with spin-orbit coupling. Physical Review B, 2012, 85, .	3.2	4
85	Remarkable Thermal Contraction in Small Size Single-Walled Boron Nanotubes. Communications in Computational Physics, 2014, 16, 201-212.	1.7	4
86	Systematic search of conformations of five tetrapeptides and a divide and conquer strategy for the predictions of peptide structures. Computational and Theoretical Chemistry, 2017, 1108, 40-49.	2.5	4
87	Structural Information-Based Method for the Efficient and Reliable Prediction of Oligopeptide Conformations. Journal of Physical Chemistry B, 2017, 121, 2525-2533.	2.6	4
88	Computational study on single molecular spectroscopy of tyrosin-glycine, tryptophane-glycine and glycine-tryptophane. Scientific Reports, 2017, 7, 15869.	3.3	4
89	Theoretical prediction of a highly responsive material: Spin fluctuations and superconductivity in FeNiB2 system. Applied Physics Letters, 2019, 115, 182601.	3.3	4
90	Multiscale Catalyst Design for Steam Methane Reforming Assisted by Deep Learning. Journal of Physical Chemistry C, 2021, 125, 10860-10867.	3.1	4

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91	How to Look for Compounds: Predictive Screening and in situ Studies in Na ⁺ Zn ²⁺ Bi System. Chemistry - A European Journal, 2021, 27, 15954-15966.	3.3	4
92	Catalytic Effect of Hydrogen Bond on Oxhydryl Dehydrogenation in Methanol Steam Reforming on Ni(111). Molecules, 2020, 25, 1531.	3.8	3
93	Genetic Algorithm Embedded with a Search Space Dimension Reduction Scheme for Efficient Peptide Structure Predictions. Journal of Physical Chemistry B, 2021, 125, 3824-3829.	2.6	3
94	Deposition and growth kinetics studies of thin zirconium dioxide films by UVILS-CVD. Applied Surface Science, 2007, 253, 7942-7946.	6.1	2
95	Extensive Computational Study on Conformations of Microsolvated Leucine Complexes. Chinese Journal of Chemical Physics, 2012, 25, 409-418.	1.3	2
96	Intermolecular π/π and H/ π interactions in dimers researched by different computational methods. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450057.	1.8	2
97	Stabilizing reconstruction induced by O protrusions of the ZnO (0001) polar surface. RSC Advances, 2014, 4, 54249-54255.	3.6	2
98	A comparative study of Sm networks in Al-10 at.%Sm glass and associated crystalline phases. Philosophical Magazine Letters, 2018, 98, 27-37.	1.2	2
99	A random forest learning assisted α -divide and conquer approach for peptide conformation search. Scientific Reports, 2018, 8, 8796.	3.3	2
100	Electronic structures of intermolecular hydrogen bond contacts with solute in aqueous solution: glycine as a working prototype. Physical Chemistry Chemical Physics, 2016, 18, 15894-15898.	2.8	1
101	Theoretical Modeling for Fundamental Understanding of High-Temperature Solid Oxide Fuel Cells. Electrochemical Energy Storage and Conversion, 2015, , 339-361.	0.0	0
102	Combining classical molecular docking with self-consistent charge density-functional tight-binding computations for the efficient and quality prediction of ligand binding structure. Journal of Chemical Research, 2022, 46, 174751982211019.	1.3	0
103	Analysis of the sidechain structures of amino acids and peptides and a deduced method for the efficient search of peptide conformations. Computational and Theoretical Chemistry, 2022, 1215, 113815.	2.5	0
104	Extensive exploration of the conformational landscapes of neutral and terminally blocked prolines in the gas phase: A density functional theory study. Journal of Chemical Research, 2022, 46, 174751982211104.	1.3	0