Zijing Lin

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2045551/publications.pdf

Version: 2024-02-01

104	2,716	147801	206112
papers	citations	31 h-index	48 g-index

104	104	104	2177
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	Effects of methane steam reforming on the mechanical stability of solid oxide fuel cell stack. Applied Energy, 2022, 322, 119464.	10.1	11
3	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
4	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
5	Parametric study of kW-class solid oxide fuel cell stacks fueled by hydrogen and methane with fully multiphysical coupling model. International Journal of Hydrogen Energy, 2021, 46, 9488-9502.	7.1	26
6	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
7	Multiscale Catalyst Design for Steam Methane Reforming Assisted by Deep Learning. Journal of Physical Chemistry C, 2021, 125, 10860-10867.	3.1	4
8	Ternary Zinc Antimonides Unlocked Using Hydride Synthesis. Inorganic Chemistry, 2021, 60, 10686-10697.	4.0	6
9	Long-term evolution of mechanical performance of solid oxide fuel cell stack and the underlying mechanism. International Journal of Hydrogen Energy, 2021, 46, 24293-24304.	7.1	16
10	Continuum scale modelling and complementary experimentation of solid oxide cells. Progress in Energy and Combustion Science, 2021, 85, 100902.	31.2	58
11	How to Look for Compounds: Predictive Screening and inâ€…situ Studies in Naâˆ’Znâˆ’Bi System. Chemistry - A European Journal, 2021, 27, 15954-15966.	3.3	4
12	Optimization Design of Rib Width and Performance Analysis of Solid Oxide Electrolysis Cell. Energies, 2020, 13, 5468.	3.1	9
13	Stabilizing the crystal structures of NaFePO₄ with Li substitutions. Physical Chemistry Chemical Physics, 2020, 22, 13975-13980.	2.8	8
14	Theoretical search for possible Liâ€“Niâ€“B crystal structures using an adaptive genetic algorithm. Journal of Applied Physics, 2020, 127, .	2.5	8
15	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
16	Density Functional Theory Based Micro- and Macro-Kinetic Studies of Ni-Catalyzed Methanol Steam Reforming. Catalysts, 2020, 10, 349.	3.5	5
17	Catalytic Effect of Hydrogen Bond on Oxhydryl Dehydrogenation in Methanol Steam Reforming on Ni(111). Molecules, 2020, 25, 1531.	3.8	3
18	Theoretical prediction of a highly responsive material: Spin fluctuations and superconductivity in FeNiB2 system. Applied Physics Letters, 2019, 115, 182601.	3.3	4

#	Article	IF	Citations
19	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
20	Feâ€“Si networks and charge/discharge-induced phase transitions in Li₂FeSiO₄ cathode materials. Physical Chemistry Chemical Physics, 2018, 20, 14557-14563.	2.8	12
21	Degradations of the electrochemical performance of solid oxide fuel cell induced by material microstructure evolutions. Applied Energy, 2018, 231, 22-28.	10.1	40
22	A random forest learning assisted â€œdivide and conquerâ€•approach for peptide conformation search. Scientific Reports, 2018, 8, 8796.	3.3	2
23	Numerical study on the mechanical stress and mechanical failure of planar solid oxide fuel cell. Applied Energy, 2018, 229, 63-68.	10.1	49
24	Effects of Electrode Composition and Thickness on the Mechanical Performance of a Solid Oxide Fuel Cell. Energies, 2018, 11, 1735.	3.1	47
25	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
26	A scheme for the generation of Feâ€“P networks to search for low-energy LiFePO4 crystal structures. Journal of Materials Chemistry A, 2017, 5, 14611-14618.	10.3	9
27	A multiphysics fully coupled modeling tool for the design and operation analysis of planar solid oxide fuel cell stacks. Applied Energy, 2017, 190, 1234-1244.	10.1	75
28	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
29	Computational study on single molecular spectroscopy of tyrosin-glycine, tryptophane-glycine and glycine-tryptophane. Scientific Reports, 2017, 7, 15869.	3.3	4
30	A theoretical framework for multiphysics modeling of methane fueled solid oxide fuel cell and analysis of low steam methane reforming kinetics. Applied Energy, 2016, 176, 1-11.	10.1	37
31	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
32	A genetic algorithm encoded with the structural information of amino acids and dipeptides for efficient conformational searches of oligopeptides. Journal of Computational Chemistry, 2016, 37, 1214-1222.	3.3	9
33	Heat transfer in the dynamic cycling of lithiumâ€“titanate batteries. International Journal of Heat and Mass Transfer, 2016, 93, 896-905.	4.8	69
34	Theoretical Modeling for Fundamental Understanding of High-Temperature Solid Oxide Fuel Cells. Electrochemical Energy Storage and Conversion, 2015, , 339-361.	0.0	0
35	Exploration of tetrahedral structures in silicate cathodes using a motif-network scheme. Scientific Reports, 2015, 5, 15555.	3.3	27
36	Theoretical spectroscopic studies on chemical and electronic structures of arginylglycine. Physical Chemistry Chemical Physics, 2015, 17, 24754-24760.	2.8	7

#	Article	IF	Citations
37	Intermolecular Ï€/Ï€ and H/Ï€ interactions in dimers researched by different computational methods. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450057.	1.8	2
38	The role of dimerization on the structure transformation of arginine in gas phase. Chemical Physics Letters, 2014, 608, 398-403.	2.6	7
39	Pure valley current generation in graphene with a Dirac gap by quantum pumping. Applied Physics Express, 2014, 7, 125102.	2.4	17
40	Quantum pumping of valley current in strain engineered graphene. Applied Physics Letters, 2014, 104, .	3.3	42
41	Stabilizing reconstruction induced by O protrusions of the ZnO (0001) polar surface. RSC Advances, 2014, 4, 54249-54255.	3.6	2
42	A Schottky barrier based model for the grain size effect on oxygen ion conductivity of acceptor-doped ZrO2 and CeO2. International Journal of Hydrogen Energy, 2014, 39, 14334-14341.	7.1	19
43	Gas-phase IR spectroscopy of deprotonated amino acids: Global or Local minima?. Chemical Physics Letters, 2014, 598, 86-90.	2.6	18
44	Theoretical models for effective electrical and electrochemical properties of nano-particle infiltrated electrode of solid oxide fuel cell. International Journal of Hydrogen Energy, 2014, 39, 15982-15988.	7.1	9
45	Complexations of alkali/alkaline earth metal cations with gaseous glutamic acid. Computational and Theoretical Chemistry, 2014, 1039, 1-10.	2.5	9
46	Point defect weakened thermal contraction in monolayer graphene. Journal of Chemical Physics, 2014, 141, 064705.	3.0	11
47	A fragment based step-by-step strategy for determining the most stable conformers of biomolecules. Chemical Physics Letters, 2014, 610-611, 303-309.	2.6	13
48	Property models and theoretical analysis of novel solid oxide fuel cell with triplet nano-composite electrode. International Journal of Hydrogen Energy, 2014, 39, 13763-13769.	7.1	8
49	Theoretical model for surface diffusion driven Ni-particle agglomeration in anode of solid oxide fuel cell. Journal of Power Sources, 2014, 255, 144-150.	7.8	29
50	Remarkable Thermal Contraction in Small Size Single-Walled Boron Nanotubes. Communications in Computational Physics, 2014, 16, 201-212.	1.7	4
51	Thorough theoretical search of conformations of neutral, protonated and deprotonated glutamine in gas phase. Computational and Theoretical Chemistry, 2013, 1020, 14-21.	2.5	11
52	Theoretical studies on the electrochemical and mechanical properties and microstructure optimization of micro-tubular solid oxide fuel cells. Journal of Power Sources, 2013, 232, 106-122.	7.8	34
53	Zwitterions are the most stable form for neutral arginylglycine in gas phase: Clear theoretical evidence. Computational and Theoretical Chemistry, 2013, 1008, 96-102.	2.5	9
54	Spin polarization switching in monolayer graphene through a Rashba multi-barrier structure. Applied Physics Letters, 2013, 102, .	3.3	18

#	Article	IF	Citations
55	Spin transport in graphene spinâ€“orbit barrier structure. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 632-636.	2.1	13
56	Extensive Computational Study on Conformations of Microsolvated Leucine Complexes. Chinese Journal of Chemical Physics, 2012, 25, 409-418.	1.3	2
57	Transverse currents in triplet Josephson junction with spin-orbit coupling. Physical Review B, 2012, 85, .	3.2	4
58	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
59	Generation of large spin currents in graphene using adiabatic quantum pumping. Journal of Applied Physics, 2012, 112, 073701.	2.5	8
60	Inducing extended line defects in graphene by linear adsorption of C and N atoms. Applied Physics Letters, 2012, 101, .	3.3	7
61	First-Principles Study on Core-Level Spectroscopy of Arginine in Gas and Solid Phases. Journal of Physical Chemistry B, 2012, 116, 12641-12650.	2.6	23
62	Comprehensive Conformational Studies of Five Tripeptides and a Deduced Method for Efficient Determinations of Peptide Structures. Journal of Physical Chemistry B, 2012, 116, 2269-2283.	2.6	17
63	Atomic nitrogen chemisorption on graphene with extended line defects. Journal of Materials Chemistry, 2012, 22, 21167.	6.7	14
64	Extensive Computational Study on Coordination of Transition Metal Cations and Water Molecules to Glutamic Acid. Journal of Physical Chemistry A, 2012, 116, 7177-7188.	2.5	10
65	Effects of electrode composition on the electrochemical performance and mechanical property of micro-tubular solid oxide fuel cell. International Journal of Hydrogen Energy, 2012, 37, 12925-12940.	7.1	44
66	Adsorption and properties of aromatic amino acids on single-walled carbon nanotubes. Nanoscale, 2012, 4, 1146-1153.	5.6	45
67	The influence of interconnect ribs on the performance of planar solid oxide fuel cell and formulae for optimal rib sizes. Journal of Power Sources, 2012, 204, 106-115.	7.8	67
68	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. Journal of Power Sources, 2012, 206, 171-178.	7.8	70
69	Comprehensive computational study of gas-phase conformations of neutral, protonated and deprotonated glutamic acids. Computational and Theoretical Chemistry, 2011, 976, 42-50.	2.5	23
70	Conformational search for zwitterionic leucine and hydrated conformers of both the canonical and zwitterionic leucine using the DFT-CPCM model. Vibrational Spectroscopy, 2011, 56, 74-81.	2.2	19
71	Spin current generation by adiabatic pumping in monolayer graphene. Applied Physics Letters, 2011, 98, .	3.3	59
72	Flow uniformity optimization for large size planar solid oxide fuel cells with U-type parallel channel designs. Journal of Power Sources, 2010, 195, 3207-3214.	7.8	28

#	Article	IF	Citations
73	Combined micro-scale and macro-scale modeling of the composite electrode of a solid oxide fuel cell. Journal of Power Sources, 2010, 195, 6598-6610.	7.8	66
74	Comprehensive ab initio study on the conformations of L-Threonine and L-allo-Threonine and related species in gas phase. Computational and Theoretical Chemistry, 2010, 962, 23-32.	1.5	19
75	Comprehensive Density Functional Theory Study on the Mechanism of Activation of the Nonapeptide Hormone Oxytocin by Metal Ions. Journal of Physical Chemistry B, 2010, 114, 1417-1423.	2.6	14
76	A Microscale Modeling Tool for the Design and Optimization of Solid Oxide Fuel Cells. Energies, 2009, 2, 427-444.	3.1	22
77	Comparison of some representative density functional theory and wave function theory methods for the studies of amino acids. Journal of Computational Chemistry, 2009, 30, 589-600.	3.3	61
78	Extensive conformational searches of 13 representative dipeptides and an efficient method for dipeptide structure determinations based on amino acid conformers. Journal of Computational Chemistry, 2009, 30, 2105-2121.	3.3	32
79	Structural stabilities of metalated histidines in gas phase and existence of gaseous zwitterionic histidine conformers. Computational and Theoretical Chemistry, 2009, 895, 65-71.	1.5	20
80	Effects of microsolvation and aqueous solvation on the tautomers of histidine: a computational study on energy, structure and IR spectrum. Theoretical Chemistry Accounts, 2009, 124, 37-47.	1.4	27
81	A key geometric parameter for the flow uniformity in planar solid oxide fuel cell stacks. International Journal of Hydrogen Energy, 2009, 34, 3873-3884.	7.1	78
82	Percolation theory to predict effective properties of solid oxide fuel-cell composite electrodes. Journal of Power Sources, 2009, 191, 240-252.	7.8	176
83	Three-dimensional modeling of planar solid oxide fuel cells and the rib design optimization. Journal of Power Sources, 2009, 194, 854-863.	7.8	62
84	An exploration of conformational search of leucine molecule and their vibrational spectra in gas phase using ab initio methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 73, 865-870.	3.9	22
85	The effects of the interconnect rib contact resistance on the performance of planar solid oxide fuel cell stack and the rib design optimization. Journal of Power Sources, 2008, 183, 214-225.	7.8	90
86	A semi-empirical and ab initio combined approach for the full conformational searches of gaseous lysine and lysineâ€“H2O complex. Computational and Theoretical Chemistry, 2008, 858, 52-65.	1.5	39
87	Ab initiostudies of aspartic acid conformers in gas phase and in solution. Journal of Chemical Physics, 2007, 127, 154314.	3.0	44
88	Protonation Processes and Electronic Spectra of Histidine and Related Ions. Journal of Physical Chemistry A, 2007, 111, 4340-4352.	2.5	61
89	Deposition and growth kinetics studies of thin zirconium dioxide films by UVILS-CVD. Applied Surface Science, 2007, 253, 7942-7946.	6.1	2
90	Gaseous Arginine Conformers and Their Unique Intramolecular Interactions. Journal of Physical Chemistry A, 2006, 110, 12282-12291.	2.5	100

#	Article	IF	Citations
91	Exploration of the full conformational landscapes of gaseous aromatic amino acid phenylalanine: An ab initio study. Computational and Theoretical Chemistry, 2006, 758, 195-202.	1.5	70
92	Ab initio studies of the conformers and conformational distribution of the gaseous hydroxyamino acid threonine. Computational and Theoretical Chemistry, 2006, 760, 159-166.	1.5	27
93	First-principle studies of gaseous aromatic amino acid histidine. Computational and Theoretical Chemistry, 2006, 801, 7-20.	1.5	35
94	Coexistence of Dihydrogen, Blue- and Red-Shifting Hydrogen Bonds in an Ultrasmall System: Valine. ChemPhysChem, 2006, 7, 828-830.	2.1	40
95	Ab initio studies of gas phase asparagine conformers. Computational and Theoretical Chemistry, 2005, 719, 153-158.	1.5	32
96	Detailed Ab Initio Studies of the Conformers and Conformational Distributions of Gaseous Tryptophan. Journal of Physical Chemistry A, 2005, 109, 2656-2659.	2.5	75
97	Systematic ab initio studies of the conformers and conformational distribution of gas-phase tyrosine. Journal of Chemical Physics, 2005, 122, 134313.	3.0	62
98	The effect of interconnect rib size on the fuel cell concentration polarization in planar SOFCs. Journal of Power Sources, 2003, 117, 92-97.	7.8	61
99	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
100	LDA and GGA calculations of alkali metal adsorption at the (001) surface of MgO. Journal of Chemical Physics, 2000, 112, 3014-3022.	3.0	38
101	Adsorption of CO on MgO supported alkali monolayers: a periodic density functional local density approximation and generalized gradient approximation study. Surface Science, 2000, 445, 495-505.	1.9	18
102	Multicenter Integration Scheme for Electronic Structure Calculations of Periodic and Nonperiodic Polyatomic Systems. Journal of Physical Chemistry A, 1999, 103, 2117-2127.	2.5	16
103	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
104	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