Xinlu Cheng

List of Publications by Year
in descending order

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48	547	623734	677142
papers	citations	14	22
		h-index	g-index

48	48	48	713
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electronic and magnetic properties of all 3d transitionâ€metalâ€doped ZnO monolayers. International Journal of Quantum Chemistry, 2013, 113, 2243-2250.	2.0	88
2	The Correlation between Electric Spark Sensitivity of Polynitroaromatic Compounds and Their Molecular Electronic Properties. Propellants, Explosives, Pyrotechnics, 2010, 35, 555-560.	1.6	41
3	Phase transition and elasticity of CdO under pressure. Physica Status Solidi (B): Basic Research, 2009, 246, 71-76.	1.5	35
4	Responses of Coreâ€“Shell Al/Al₂O₃ Nanoparticles to Heating: ReaxFF Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2018, 122, 9191-9197.	3.1	34
5	Firstâ€principles calculations on elasticity and the thermodynamic properties of TaC under pressure. Physica Status Solidi (B): Basic Research, 2009, 246, 1590-1596.	1.5	28
6	ReaxFF Molecular Dynamics Study of Initial Mechanism of JP-10 Combustion. Combustion Science and Technology, 2012, 184, 1233-1243.	2.3	26
7	DFT Study of Solvent Effects for Some Organic Molecules Using a Polarizable Continuum Model. Journal of Solution Chemistry, 2006, 35, 869-878.	1.2	22
8	Effect of electric field on polarization and decomposition of RDX molecular crystals: a ReaxFF molecular dynamics study. Journal of Molecular Modeling, 2020, 26, 2.	1.8	20
9	The Câ”NO2 bond dissociation energies of some nitroaromatic compounds: DFT study. Structural Chemistry, 2006, 17, 547-550.	2.0	19
10	MOLECULAR DYNAMIC SIMULATIONS OF SOLID NITROMETHANE UNDER HIGH PRESSURES. Journal of Theoretical and Computational Chemistry, 2010, 09, 315-325.	1.8	19
11	Theoretical calculation of bond dissociation energies and heats of formation for nitromethane and polynitromethanes with density functional theory. International Journal of Quantum Chemistry, 2007, 107, 515-521.	2.0	18
12	Prediction for electronic, vibrational and thermoelectric properties of chalcopyrite AgX(X=In,Ga)Te ₂ : PBEâ€‰+â€‰U approach. Royal Society Open Science, 2017, 4, 170750.	2.4	17
13	Calculations of the Bond Dissociation Energies for NO2 Scission in Some Nitro Compounds. Structural Chemistry, 2005, 16, 457-460.	2.0	16
14	Phase transition, and elastic and thermodynamic properties of InN derived from firstâ€principles and the quasiâ€harmonic Debye model. Physica Status Solidi (B): Basic Research, 2008, 245, 2743-2748.	1.5	15
15	Lattice instability of V2AlC at high pressure. Science China: Physics, Mechanics and Astronomy, 2013, 56, 916-924.	5.1	13
16	Quantum Chemical Study on the Interactions of NO₃ with RDX and Four Decomposition Intermediates. Propellants, Explosives, Pyrotechnics, 2010, 35, 315-320.	1.6	12
17	The mechanical and thermal responses of colliding oxide-coated aluminum nanoparticles. Journal of Applied Physics, 2017, 121, .	2.5	11
18	Ab initio simulation of laser-induced water decomposition close to carbon nanotubes. Physical Review B, 2019, 99, .	3.2	10

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19	Firstâ€principles calculations of transition phase and thermodynamic properties of CdO. Physica Status Solidi (B): Basic Research, 2008, 245, 1113-1117.	1.5	9
20	Bond dissociation energies for removal of the hydroxyl group in some alcohols from quantum chemical calculations. International Journal of Quantum Chemistry, 2012, 112, 665-671.	2.0	8
21	Ab initio calculation of the thermodynamic properties of InSb under intense laser irradiation. Journal of Applied Physics, 2013, 114, 043519.	2.5	7
22	Theoretical study of spectral parameters for the Î³ and Î² band systems of NO for atmosphere and high temperature. Molecular Physics, 2017, 115, 2577-2585.	1.7	7
23	Theoretical Study on Electronic, Optical Properties and Hardness of Technetium Phosphides under High Pressure. Crystals, 2017, 7, 176.	2.2	7
24	A first-principles investigation into the hydrogen bond interaction in Î²-HMX. Science China: Physics, Mechanics and Astronomy, 2010, 53, 1080-1085.	5.1	6
25	Diffusion monte carlo study of the hydrogen molecules adsorbed on C₄H₃Li. International Journal of Quantum Chemistry, 2012, 112, 2627-2631.	2.0	6
26	A timeâ€dependent density functional study on optical response in allâ€inorganic leadâ€halide perovskite nanostructures. International Journal of Quantum Chemistry, 2020, 120, e26232.	2.0	6
27	Electron-impact high-lying <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow><mml:mo>â^'</mml:mo></mml:msup></mml:m resonant states. Physical Review A, 2022, 105, .	2.5	6
28	Bond covalency and electronic structure of CaB2O4(III) crystal. Structural Chemistry, 2009, 20, 221-226.	2.0	5
29	Al-doped graphene as an effective adsorber for some toxic derivatives of aromatic hydrocarbons. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750004.	1.8	5
30	The mystery of abnormally large volume of PbCrO3 with a structurally consistent Hubbard U from first-principles. European Physical Journal B, 2013, 86, 1.	1.5	4
31	Phase transition and elastic properties of NbN under hydrostatic pressure. Journal Wuhan University of Technology, Materials Science Edition, 2014, 29, 49-57.	1.0	4
32	Phase Transition and Chemical Decomposition of Liquid Oxygen and Nitrogen Mixture under High Pressures. Journal of Physical Chemistry C, 2016, 120, 13366-13374.	3.1	4
33	Ab initio study: the potential energy curves and ro-vibrational spectrum of low-lying excited states of HCl⁺ cation. Molecular Physics, 2016, 114, 2817-2823.	1.7	3
34	First-principles study of Li decorated coronene graphene. International Journal of Modern Physics B, 2017, 31, 1750216.	2.0	3
35	STRUCTURAL AND ELECTRONIC PROPERTIES OF Sr(N₃)₂ UNDER PRESSURE. Journal of Theoretical and Computational Chemistry, 2007, 06, 487-494.	1.8	2
36	A TDDFT Investigation on Plasmons in Multilayer Graphene Nanostructures. Plasmonics, 2017, 12, 1967-1973.	3.4	2

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37	State-to-State Transition Study of the Exchange Reaction for N(⁴S) and O₂(X³Σ_g^{â¯}) Collision by Quasi-Classical Trajectory. Journal of Physical Chemistry A, 2021, 125, 9318-9326.	2.5	2
38	State-Specific Dynamic Study of the Exchange and Dissociation Reaction for O(3P) and O2($${}^{3}Sigma _{g}^{ - }$$) Collision by Quasi-Classical Trajectory. Russian Journal of Physical Chemistry A, 2022, 96, 876-883.	0.6	2
39	Density functional theoretical study on attachment sites of Mg2+ and Ca2+ and metal ion affinity to Crenulatin molecule. Structural Chemistry, 2008, 19, 541-548.	2.0	1
40	AB INITIO CALCULATIONS OF STRUCTURAL AND ELECTRONIC PROPERTIES OF THE COMPOUND Li3AlB2O6. Modern Physics Letters B, 2008, 22, 343-352.	1.9	1
41	Inelastic partial cross sections for scattering of HF by neon. Science in China Series G: Physics, Mechanics and Astronomy, 2009, 52, 574-579.	0.2	1
42	Ab initio study of the structures and hydrogen storage capacity of (H₂)_nCH₄ compound. Modern Physics Letters B, 2015, 29, 1550062.	1.9	1
43	Regulation of Nb3+, Sb3+ and V3+ doping on the photo-induced ferroelectricity of KTaO3. Physica B: Condensed Matter, 2021, 620, 413248.	2.7	1
44	Theoretical investigation on heats of formation for derivatives of 1,2,4-triazole. , 2011, , .		0
45	Theoretical study on the interaction between C₃ molecular wires and nanotubes. Physica Status Solidi (B): Basic Research, 2011, 248, 1464-1470.	1.5	0
46	Collision-Induced Rotational Excitation of CO2 by N(4S) Atoms: A New Ab Initio Potential Energy Surface and Scattering Calculations. Journal of Physical Chemistry A, 2021, 125, 1134-1141.	2.5	0
47	Modulation of Oxygen Vacancy on Midinfrared Lightâ€Induced Ferroelectricity of KTaO 3. Physica Status Solidi (B): Basic Research, 2021, 258, 2100099.	1.5	0
48	R-Matrix Calculation of Electron Collisions with Molecular Oxygen in Its Electronically Excited States. Journal of Physical Chemistry A, 2022, 126, 2061-2074.	2.5	0