

Xiaojun Li

List of Publications by Year in descending order

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Version: 2024-02-01

26
papers

719
citations

567281

15
h-index

580821

25
g-index

26
all docs

26
docs citations

26
times ranked

732
citing authors

#	ARTICLE	IF	CITATIONS
1	Computational study of oxidation mechanism of mineral green pigments. <i>Journal of Molecular Modeling</i> , 2021, 27, 108.	1.8	0
2	Activation of adenosine A3 receptor reduces early brain injury by alleviating neuroinflammation after subarachnoid hemorrhage in elderly rats. <i>Aging</i> , 2021, 13, 694-713.	3.1	16
3	Remarkably enhanced first hyperpolarizability and nonlinear refractive index of novel graphdiyne-based materials for promising optoelectronic applications: A first-principles study. <i>Applied Surface Science</i> , 2020, 512, 145544.	6.1	38
4	Exploring the influence of water molecules on the stability of the cinnabar oxides. <i>Chemical Physics Letters</i> , 2020, 747, 137351.	2.6	2
5	Structures, electronic properties, hydration and UV-vis absorption spectra of actinide motexafins [An-Motex] ₂ ⁺ (An = Ac, Cm, Lr) and [UO ₂ -Motex] ₁ ⁺ : insights from DFT calculations. <i>Molecular Physics</i> , 2020, 118, e1736676.	1.7	1
6	The influence of water molecules on the stability of mineral green pigments in Chinese ancient painting. <i>Chemical Physics Letters</i> , 2019, 731, 136592.	2.6	5
7	Giant enhancement of electronic polarizability and the first hyperpolarizability of fluoride-decorated graphene versus graphyne and graphdiyne: insights from <i>ab initio</i> calculations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 13165-13175.	2.8	31
8	Investigations of electronic and nonlinear optical properties of single alkali metal adsorbed graphene, graphyne and graphdiyne systems by first-principles calculations. <i>Journal of Materials Chemistry C</i> , 2019, 7, 1630-1640.	5.5	101
9	Systematic Theoretical Study of Electronic Structures and Stability of Transition-Metal-Adsorbed Graphdiyne Clusters. <i>Journal of Physical Chemistry C</i> , 2019, 123, 8843-8850.	3.1	20
10	Spectroscopic properties and activated mechanism of NO on isolated cationic tantalum clusters: A first-principles study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 216, 335-341.	3.9	5
11	Graphdiyne: A promising nonlinear optical material modulated by tetrahedral alkali-metal nitrides. <i>Journal of Molecular Liquids</i> , 2019, 277, 641-645.	4.9	41
12	Design of novel graphdiyne-based materials with large second-order nonlinear optical properties. <i>Journal of Materials Chemistry C</i> , 2018, 6, 7576-7583.	5.5	67
13	Structural, electronic and spectral properties of carborane-containing boron dipyrromethenes (BODIPYs): A first-principles study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 185, 149-154.	3.9	6
14	The chemical bonding and spectral assignments of rhodium(III)-catalyzed <i>closo</i> -dodecaborate complexes: <i>Ab initio</i> study. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25422.	2.0	2
15	Effect of Alkali Metal Atoms Doping on Structural and Nonlinear Optical Properties of the Gold-Germanium Bimetallic Clusters. <i>Nanomaterials</i> , 2017, 7, 184.	4.1	13
16	Cardioprotection Effects of Sevoflurane by Regulating the Pathway of Neuroactive Ligand-Receptor Interaction in Patients Undergoing Coronary Artery Bypass Graft Surgery. <i>Computational and Mathematical Methods in Medicine</i> , 2017, 2017, 1-7.	1.3	13
17	Modification of alkali metals on silicon-based nanoclusters: An enhanced nonlinear optical response. <i>Chemical Physics Letters</i> , 2016, 659, 93-99.	2.6	30
18	Deferoxamine pre-treatment protects against postoperative cognitive dysfunction of aged rats by depressing microglial activation via ameliorating iron accumulation in hippocampus. <i>Neuropharmacology</i> , 2016, 111, 180-194.	4.1	33

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19	The nature of structure and bonding between transition metal and mixed Siâ€¢Ge tetramers: A 20â€¢electron superatom system. <i>Journal of Computational Chemistry</i> , 2016, 37, 2316-2323.	3.3	27
20	Deferoxamine regulates neuroinflammation and iron homeostasis in a mouse model of postoperative cognitive dysfunction. <i>Journal of Neuroinflammation</i> , 2016, 13, 268.	7.2	83
21	Propofol postsynaptically suppresses stellate neuron excitability in the entorhinal cortex by influencing the HCN and TREK-2 channels. <i>Neuroscience Letters</i> , 2016, 619, 54-59.	2.1	5
22	Exploring the chemical bonding, infrared and UVâ€¢vis absorption spectra of OH radicals adsorption on the smallest fullerene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 144, 258-265.	3.9	15
23	Determination of Absolute Configuration and Conformation of a Cyclic Dipeptide by NMR and Chiral Spectroscopic Methods. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1721-1736.	2.5	59
24	Transferability of Various Molecular Property Tensors in Vibrational Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 977-985.	5.3	60
25	Absolute Configuration of a Cyclic Dipeptide Reflected in Vibrational Optical Activity: Ab Initio and Experimental Investigation. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2554-2563.	2.5	30
26	Theoretical study on the smallest endohedral metallofullerenes: TM@C₂₀ (TM = Ce and Tj). <i>Journal of Physical Chemistry A</i> , 2012, 116, 10100-10106.	2.8	16