Jucai Yang

List of Publications by Year
in descending order

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45	590	623734	677142
papers	citations	14 h-index	22 g-index

46	46	46	328
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theoretical Study on Structural Stability, Growth Behavior and Photoelectron Spectroscopy of Copper-Doped Germanium Clusters CuGenâ^'/0 (nâ€‰=â€‰4â€“13). Journal of Cluster Science, 2022, 33, 403-412.	3.3	3
2	A systematic investigation of structural growth patterns and electronic properties of [LuGe]+/0 and [Ge+1]+/0 (nÂ=Â1â€“17) nanoalloy clusters. Materials Today Communications, 2022, 30, 103018.	1.9	3
3	Optimized nonlinear optical (NLO) response of silicon carbide nanosheet by alkali metals doping: a DFT insight. European Physical Journal Plus, 2022, 137, 1.	2.6	23
4	Europiumâ€linked structures and electronic properties of nanosize semiconductor <scp>EuSi_n⁰</scp>^{/â^'} (n = 11â€18) clusters. International Journal of Quantum Chemistry, 2021, 121, e26457.	2.0	4
5	Study on the growth behavior and photoelectron spectroscopy of neodymium-doped silicon nanoclusters NdSin0/â^' (nâ€‰=â€‰8â€“20) with a double-hybrid density functional theory. Journal of Molecular Modeling, 2021, 27, 86.	1.8	2
6	Comparative research of configuration, stability and electronic properties of cationic and neutral [AuGe] and [Ge+1]Î» (n=1-13, Î»=0, +1) nanoalloy clusters. Materials Today Communications, 2021, 26, 101989.	1.9	9
7	Thermochemical Properties and Growth Mechanism of the Ag-Doped Germanium Clusters, AgGe_n^{Î»} with n = 1â€“13 and Î» = â^'1, 0, and +1. ACS Omega, 2021, 6, 9813-9827.	3.5	6
8	Theoretical exploration of global minima, magnetism, structural stability and growth pattern of holmiumâ€doped silicon HoSi n 0 /â^' (n Â=Â10â€“18) nanoclusters. International Journal of Quantum Chemistry, 2021, 121, e26776.	2.0	1
9	Unraveling the Mechanism of Aerobic Alcohol Oxidation by a Cu/pytl-Î²-Cyclodextrin/TEMPO Catalytic System under Air in Neat Water. Inorganic Chemistry, 2021, 60, 14132-14141.	4.0	4
10	Structural Evolution, Electronic Structures, and Vibrational Properties of Anionic LuGe_n (n = 5â€“17) Clusters: From Lu-Linked to Lu-Encapsulated Configurations. Inorganic Chemistry, 2021, 60, 14446-14456.	4.0	10
11	Structural stability and evolution of terbiumâ€doped silicon clusters and influence of 4fâ€‰â†'â€‰5d electronic transition mechanism on magnetism and appearance of photoelectron spectroscopy for TbSi_n^{0/â^'} (n = 6â€18) clusters. International Journal of Quantum Chemistry, 2020, 120, e26087.	2.0	9
12	Probing the electronic structures and properties of neutral and charged FeSin(â^'1,0,+1) (nâ€‰=â€‰1â€“6) clusters using ccCA theory. Journal of Molecular Modeling, 2020, 26, 283.	1.8	3
13	Facile synthesis of oxygen-deficient nano-TiO₂coordinated by acetate ligands for enhanced visible-light photocatalytic performance. Catalysis Science and Technology, 2020, 10, 3875-3889.	4.1	11
14	In-situ formation of carboxylate species on TiO2 nanosheets for enhanced visible-light photocatalytic performance. Journal of Colloid and Interface Science, 2020, 577, 512-522.	9.4	12
15	Facile synthesis of multi-type carbon doped and modified nano-TiO₂ for enhanced visible-light photocatalysis. RSC Advances, 2020, 10, 43193-43203.	3.6	2
16	Structural growth pattern of neutral and negatively charged yttrium-doped silicon clusters YSi_n^{0/â^'} (n=6â€“20): from linked to encapsulated structures. RSC Advances, 2019, 9, 2731-2739.	3.6	15
17	Study on Structural Evolution, Thermochemistry and Electron Affinity of Neutral, Mono- and Di-Anionic Zirconium-Doped Silicon Clusters ZrSin0/-/2- (n = 6â€“16). International Journal of Molecular Sciences, 2019, 20, 2933.	4.1	9
18	Revisiting the structural and electronic properties of neutral, monoâ€and diâ€anionic titaniumâ€doped silicon clusters TiSi n 0/â^'/2â^' (n = 6â€16). International Journal of Quantum Chemistry, 2019, 119, e25978.	2.0	5

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19	Theoretical Study on the Growth Behavior and Photoelectron Spectroscopy of Lanthanum-Doped Silicon Clusters LaSi n 0/â^' (nâ€‰=â€‰6â€“20). Journal of Cluster Science, 2019, 30, 789-796.	3.3	13
20	Structural and electronic properties of nanosize semiconductor CeSi0/â^' (nâ€¯=â€¯4â€“20) material: A double-hybrid density functional theory investigation. Computational and Theoretical Chemistry, 2019, 1170, 112635.	2.5	7
21	Probing Structure, Thermochemistry, Electron Affinity and Magnetic Moment of Erbium-Doped Silicon Clusters ErSin (nÂ=Â3â€“10) and Their Anions with Density Functional Theory. Journal of Cluster Science, 2018, 29, 301-311.	3.3	14
22	Mechanism of Aerobic Alcohol Oxidation Mediated by Waterâ€Soluble Cu^{II}â€TEMPO Catalyst in Water: A Density Functional Theory Study. ChemistrySelect, 2018, 3, 1268-1274.	1.5	3
23	Probing structure, thermochemistry, electron affinity, and magnetic moment of thulium-doped silicon clusters TmSi n (nâ€‰=â€‰3â€“10) and their anions with density functional theory. Journal of Molecular Modeling, 2018, 24, 29.	1.8	9
24	A new natural layered clay mineral applicable to photocatalytic hydrogen production and/or degradation of dye pollutant. Environmental Progress and Sustainable Energy, 2018, 37, 1003-1010.	2.3	11
25	Structural Stability and Evolution of Scandium-Doped Silicon Clusters: Evolution of Linked to Encapsulated Structures and Its Influence on the Prediction of Electron Affinities for ScSi_n (n = 4â€“16) Clusters. Inorganic Chemistry, 2018, 57, 12934-12940.	4.0	39
26	Study on Structure and Property of Lutetium Introduced Silicon Clusters LuSi n (nÂ=Â3â€“10) and Their Anions with Density Functional Theory. Journal of Cluster Science, 2017, 28, 2309-2322.	3.3	14
27	A direct four-electron process on Feâ€“N₃ doped graphene for the oxygen reduction reaction: a theoretical perspective. RSC Advances, 2017, 7, 23812-23819.	3.6	33
28	Density-functional study of the structures and properties of holmium-doped silicon clusters HoSi n (nâ€‰=â€‰3â€“9) and their anions. Journal of Molecular Modeling, 2017, 23, 117.	1.8	17
29	Promethium-doped silicon clusters PmSi n (nÂ=Â3â€“10) and their anions: structures, thermochemistry, electron affinities and magnetic moments. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	12
30	Stability and electronic properties of praseodymium-doped silicon clusters PrSin (nÂ=Â12â€“21). Journal of Molecular Modeling, 2017, 23, 180.	1.8	11
31	Mechanistic Insight into the 2Â° Alcohol Oxidation Mediated by an Efficient CuI/L-Proline-TEMPO Catalystâ€”A Density Functional Theory Study. Catalysts, 2017, 7, 264.	3.5	3
32	Gadolinium-doped silicon clusters GdSin (nÂ=Â2â€“9) and their anions: structures, thermochemistry, electron affinities, and magnetic moments. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	18
33	Reexamination of structures, stabilities, and electronic properties of holmium-doped silicon clusters HoSi n (nâ€‰=â€‰12â€“20). Journal of Molecular Modeling, 2016, 22, 193.	1.8	15
34	Study on the structures and properties of praseodymium-doped silicon clusters PrSi n (nÂ=Â3â€“9) and their anions with density functional schemes. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	11
35	Study on electronic structures and properties of neutral and charged arsenic sulfides [As n S3 (â^'1,0,+1), n =1â€“6] with the Gaussian-3 scheme. Journal of Molecular Modeling, 2015, 21, 303.	1.8	2
36	DFT studies on the mechanism of alcohol oxidation by the (bpy)CuI-TEMPO/NMI catalytic system. Dalton Transactions, 2015, 44, 7395-7403.	3.3	10

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37	Europium-doped silicon clusters EuSi n (nÂ=Â3â€“11) and their anions: structures, thermochemistry, electron affinities, and magnetic moments. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	30
38	Samarium doped silicon clusters SmSi (n= 3â€“10) and their anions: Structures, thermochemistry, electron affinities, and magnetic moments. Computational and Theoretical Chemistry, 2015, 1074, 1-8.	2.5	20
39	Ytterbium doped silicon clusters YbSi (n= 4â€“10) and their anions: Structures, thermochemistry, and electron affinities. Chemical Physics, 2015, 461, 11-19.	1.9	24
40	Study on structures and electronic properties of neutral and anionic TiSi_n^(0,-1)(n = 1â€“8) clusters using G4 theory. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450038.	1.8	6
41	Probing the electronic structures and properties of neutral and anionic ScSi n (0,â˜1) (nâ€‰=â€‰1â€“6) clusters using ccCA-TM and G4 theory. Journal of Molecular Modeling, 2014, 20, 2114.	1.8	15
42	Probing the electronic structures and properties of neutral and charged <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>CaSi</mml:mtext></mml:mrow><mml:mrow><mml:mi>n</mml:mi></mml:mrow> (n= 2â€“10) clusters using Gaussian-3 theory. Computational and Theoretical Chemistry, 2011, 976, 141-147.	2.5	12
43	EQUILIBRIUM GEOMETRIES AND ELECTRONIC STRUCTURE OF SMALL SILICON MONOHYDRIDES CLUSTERS. International Journal of Modern Physics B, 2006, 20, 677-695.	2.0	4
44	The small silicon clusters Sin (n=2â€“10) and their anions: structures, themochemistry, and electron affinities. Computational and Theoretical Chemistry, 2005, 719, 89-102.	1.5	85
45	Silicon Monohydride Clusters SinH (n = 4â˜10) and Their Anions:â€‰ Structures, Thermochemistry, and Electron Affinities. Journal of Physical Chemistry A, 2005, 109, 5717-5723.	2.5	19