Cheng Lu

List of Publications by Year
in descending order

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67 papers	2,062 citations	218381 26 h-index	253896 43 g-index
68 all docs	68 docs citations	68 times ranked	1289 citing authors

#	Article	IF	Citations
1	Structural Stability and Evolution of Medium-Sized Tantalum-Doped Boron Clusters: A Half-Sandwich-Structured TaB₁₂ ^{â€“} Cluster. Inorganic Chemistry, 2018, 57, 343-350.	1.9	132
2	Second group of high-pressure high-temperature lanthanide polyhydride superconductors. Physical Review B, 2020, 102, .	1.1	116
3	Elucidating Stressâ€“Strain Relations of ZrB₁₂ from First-Principles Studies. Journal of Physical Chemistry Letters, 2020, 11, 9165-9170.	2.1	97
4	Study of the Structural and Electronic Properties of Neutral and Charged Niobium-Doped Silicon Clusters: Niobium Encapsulated in Silicon Cages. Journal of Physical Chemistry C, 2016, 120, 677-684.	1.5	89
5	Hardness of FeB4: Density functional theory investigation. Journal of Chemical Physics, 2014, 140, 174505.	1.2	80
6	Systematic theoretical investigation of geometries, stabilities and magnetic properties of iron oxide clusters (FeO)_n^{Î¼}(n = 1â€“8, Î¼ = 0, Â±1): insights and perspectives. RSC Advances, 2015, 5, 6560-6570.	1.5	74
7	Insights into the geometries, electronic and magnetic properties of neutral and charged palladium clusters. Scientific Reports, 2016, 6, 19656.	1.6	73
8	Evolution of the Structural and Electronic Properties of Medium-Sized Sodium Clusters: A Honeycomb-Like Na₂₀ Cluster. Inorganic Chemistry, 2017, 56, 1241-1248.	1.9	72
9	Deciphering the Structural Evolution and Electronic Properties of Magnesium Clusters: An Aromatic Homonuclear Metal Mg₁₇ Cluster. Journal of Physical Chemistry A, 2016, 120, 7947-7954.	1.1	68
10	Dynamical behavior of boron clusters. Nanoscale, 2016, 8, 17639-17644.	2.8	67
11	Ab Initio Search for Global Minimum Structures of Pure and Boron Doped Silver Clusters. Journal of Physical Chemistry A, 2015, 119, 6738-6745.	1.1	62
12	Phase stability and superconductivity of lead hydrides at high pressure. Physical Review B, 2021, 103, .	1.1	60
13	Structural and Electronic Properties of Medium-Sized Aluminum-Doped Boron Clusters AlB_n and Their Anions. Journal of Physical Chemistry C, 2019, 123, 6276-6283.	1.5	59
14	Indentation Strengths of Zirconium Diboride: Intrinsic versus Extrinsic Mechanisms. Journal of Physical Chemistry Letters, 2021, 12, 2848-2853.	2.1	54
15	Understanding the structural transformation, stability of medium-sized neutral and charged silicon clusters. Scientific Reports, 2015, 5, 15951.	1.6	52
16	Probing the Structural Evolution and Stabilities of Medium-Sized MoB_n^{0/â€“} Clusters. Journal of Physical Chemistry C, 2018, 122, 20000-20005.	1.5	47
17	Probing the structural evolution of ruthenium doped germanium clusters: Photoelectron spectroscopy and density functional theory calculations. Scientific Reports, 2016, 6, 30116.	1.6	45
18	Prediction of Stable Ruthenium Silicides from First-Principles Calculations: Stoichiometries, Crystal Structures, and Physical Properties. ACS Applied Materials & Interfaces, 2015, 7, 26776-26782.	4.0	42

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19	Probing the low-energy structures of aluminumâ€“magnesium alloy clusters: a detailed study. Physical Chemistry Chemical Physics, 2016, 18, 26177-26183.	1.3	41
20	Indentation-strain stiffening in tungsten nitrides: Mechanisms and implications. Physical Review Materials, 2020, 4, .	0.9	41
21	Structure-strength relations of distinct MoN phases from first-principles calculations. Physical Review Materials, 2020, 4, .	0.9	41
22	Crystal Structures, Stabilities, Electronic Properties, and Hardness of MoB₂: First-Principles Calculations. Inorganic Chemistry, 2016, 55, 7033-7040.	1.9	39
23	Controlled size and morphology, and phase transition of YF₃:Yb³⁺,Er³⁺ and YOF:Yb³⁺,Er³⁺ nanocrystals for fine color tuning. Journal of Materials Chemistry C, 2016, 4, 331-339.	2.7	37
24	Structural Evolutions and Crystal Field Characterizations of Tm-Doped YAlO₃: New Theoretical Insights. ACS Applied Materials & Interfaces, 2016, 8, 30422-30429.	4.0	33
25	Negative Poisson Ratio in Two-Dimensional Tungsten Nitride: Synergistic Effect from Electronic and Structural Properties. Journal of Physical Chemistry Letters, 2020, 11, 9643-9648.	2.1	32
26	Theoretical investigation of the electronic structure and luminescence properties for Nd_xY_{1â^'x}Al₃(BO₃)₄nonlinear laser crystal. Journal of Materials Chemistry C, 2017, 5, 7174-7181.	2.7	30
27	Probing the structure and electronic properties of beryllium doped boron clusters: A planar BeB16â^' cluster motif for metallo-borophene. Scientific Reports, 2019, 9, 14367.	1.6	29
28	Structure and luminescence properties of a Nd³⁺doped Bi₄Ge₃O₁₂scintillation crystal: new insights from a comprehensive study. Journal of Materials Chemistry C, 2017, 5, 3079-3087.	2.7	27
29	Structure and Electronic Properties of Neutral and Negatively Charged RhB_n Clusters (n = 3â€“10): A Density Functional Theory Study. Journal of Physical Chemistry A, 2017, 121, 6510-6516.	1.1	24
30	Mechanical properties of tantalum carbide from high-pressure/high-temperature synthesis and first-principles calculations. Physical Chemistry Chemical Physics, 2020, 22, 5018-5023.	1.3	24
31	Deciphering the Microstructure and Energy-Level Splitting of Tm³⁺-Doped Yttrium Aluminum Garnet. Inorganic Chemistry, 2019, 58, 1058-1066.	1.9	23
32	Ternary Mg-Nb-H polyhydrides under high pressure. Physical Review B, 2021, 104, .	1.1	23
33	New Theoretical Insights into the Crystal-Field Splitting and Transition Mechanism for Nd³⁺-Doped Y₃Al₅O₁₂. ACS Applied Materials & Interfaces, 2019, 11, 10745-10750.	4.0	22
34	Insights into the Bond Behavior and Mechanical Properties of Hafnium Carbide under High Pressure and High Temperature. Inorganic Chemistry, 2021, 60, 515-524.	1.9	20
35	Pressure-Driven Structural Phase Transitions and Superconductivity of Ternary Hydride MgVH₆. Journal of Physical Chemistry C, 2021, 125, 3150-3156.	1.5	18
36	Determination of the microstructure, energy levels and magnetic dipole transition mechanism for Tm³⁺doped yttrium aluminum borate. Journal of Materials Chemistry C, 2016, 4, 1988-1995.	2.7	17

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37	A detailed investigation into the geometric and electronic structures of CoBQn (n = 2â€“10, Q = 0, â^'1) clusters. New Journal of Chemistry, 2017, 41, 11208-11214.	1.4	16
38	Prediction of Novel High-Pressure Structures of Magnesium Niobium Dihydride. ACS Applied Materials & Interfaces, 2017, 9, 26169-26176.	4.0	16
39	Exploring Physical Properties of Tantalum Carbide at High Pressure and Temperature. Inorganic Chemistry, 2020, 59, 1848-1852.	1.9	16
40	Prediction of the Iron-Based Polynuclear Magnetic Superhalogens with Pseudohalogen CN as Ligands. Inorganic Chemistry, 2017, 56, 7928-7935.	1.9	15
41	Abnormal physical behaviors of hafnium diboride under high pressure. Applied Physics Letters, 2019, 115, .	1.5	15
42	Structures, Mobilities, and Electronic Properties of Functionalized Silicene: Superhalogen BO₂ Adsorption. Inorganic Chemistry, 2020, 59, 5041-5049.	1.9	14
43	LiB13: A New Member of Tetrahedral-Typed B13 Ligand Half-Surround Cluster. Scientific Reports, 2020, 10, 1642.	1.6	14
44	Geometric Structures and Electronic Properties of AlnV0/â€“ (n = 5â€“14) Clusters: Photoelectron Spectroscopy and Theoretical Calculations. Journal of Physical Chemistry C, 2019, 123, 1931-1938.	1.5	12
45	Systematic theoretical investigation of structures, stabilities, and electronic properties of rhodium-doped silicon clusters: Rh2Si n q (nÂ=Â1â€“10; qÂ=Â0,ÂÂ±1). Journal of Materials Science, 2015, 50, 6180-6196.	1.7	11
46	Iron-based magnetic superhalogens with pseudohalogens as ligands: An unbiased structure search. Scientific Reports, 2017, 7, 45149.	1.6	11
47	Tuning of Structure Evolution and Electronic Properties through Palladium-Doped Boron Clusters: PdB₁₆ as a Motif for Boron-Based Nanotubes. Journal of Physical Chemistry A, 2020, 124, 9187-9193.	1.1	11
48	Modification of Geometric and Electronic Structures of Iron Clusters by Nitrogen: Fe8â€“ vs Fe8Nâ€“. Journal of Physical Chemistry C, 2020, 124, 3867-3872.	1.5	11
49	Exploration of stable stoichiometries, physical properties and hardness in the Rhâ€“Si system: a first-principles study. RSC Advances, 2015, 5, 53497-53503.	1.7	9
50	Insights into the Structures and Bonding of Medium-Sized Cerium-Doped Boron Clusters. Journal of Physical Chemistry A, 2021, 125, 4126-4132.	1.1	9
51	Two-Dimensional Fe₈N Nanosheets: Ferromagnets and Nitrogen Diffusion. Journal of Physical Chemistry Letters, 2021, 12, 8453-8459.	2.1	7
52	Achieving Dislocation Strengthening in Hafnium Carbide through High Pressure and High Temperature. Journal of Physical Chemistry C, 2021, 125, 24254-24262.	1.5	7
53	Theoretical investigation on the structural and thermodynamic properties of FeSe at high pressure and high temperature. Dalton Transactions, 2012, 41, 9781.	1.6	6
54	First-principles study on the geometries, stabilities and electronic properties of yttriumâ€“silicon clusters (Y2Si n ; 1Ââ‰ÂnÂâ‰Â12). Structural Chemistry, 2016, 27, 983-992.	1.0	6

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55	New insight into the structural evolution of PbTiO₃: an unbiased structure search. Physical Chemistry Chemical Physics, 2017, 19, 1420-1424.	1.3	5
56	Probing the structures, electronic and bonding properties of multidecker lanthanides: Neutral and anionic Ln (COT) (LnÂ=ÂCe,ÂNd,ÂEu, Ho and Yb; n, mÂ= 1, 2) complexes. Journal of Molecular Graphics and Modelling, 2019, 90, 226-234.	1.3	5
57	Structures, Stabilities, and Electronic Properties of Small-Sized Zr2Si n (n=1â€“11) Clusters: A Density Functional Study. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2015, 70, 805-814.	0.7	4
58	Theoretical investigation on the geometries and electronic properties of cesiumâ€“silicon CsSi n (nÂ=Â2â€“12) clusters. Structural Chemistry, 2016, 27, 457-465.	1.0	4
59	Probing the Structural and Electronic Properties of Dirhenium Halide Clusters: A Density Functional Theory Study. Scientific Reports, 2018, 8, 6702.	1.6	4
60	Structural, Stabilities, and Electronic Properties of Bimetallic Mg2-doped Silicon Clusters. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2014, 69, 481-488.	0.7	3
61	Structures and bonding of auropolyboroenes [Au₂(B₄)_xB₃]^{â¯}, [Au₂(B₄)_xB₂]^{2â¯} and [Au₂(B₄)_xB]⁺ (x = 2, 3): comparison with dihydride polyboroenes. RSC Advances, 2015, 5, 87855-87863.	1.7	3
62	Investigation on the neutral and anionic BxAlyH2 (x + y = 7, 8, 9) clusters using density functional theory combined with photoelectron spectroscopy. Physical Chemistry Chemical Physics, 2016, 18, 23296-23303.	1.3	3
63	Identification of octahedral coordinated ZrN₁₂⁺ cationic clusters by mass spectrometry and structure searches. Dalton Transactions, 2021, 50, 10187-10192.	1.6	3
64	Structural evolution and phase transition mechanism of $$hbox {MoSe}_2$$ under high pressure. Scientific Reports, 2021, 11, 22090.	1.6	3
65	Theoretical study of the structures, stabilities, and electronic properties of neutral and anionic Ca2Si n Î» (n = 1â€“8, Î» = 0, +1) clusters. European Physical Journal D, 2014, 68, 1.	0.6	2
66	Probing the structural, bonding, electronic and magnetic properties of transitionâ€“metal borazine systems: Com(borazine)n (mâ€‰=â€‰1, 2; nâ€‰=â€‰1â€“3). Molecular Physics, 2020, 118, e1667542.	0.8	1
67	Stressâ€“Strain Relations and Deformation Mechanisms of ZrN and HfN Superconductors. Crystal Growth and Design, 2022, 22, 1104-1109.	1.4	1