Cheng Lu

List of Publications by Year in Descending Order

66 papers	1,472 citations	24 h-index	36 g-index
68 ext. papers	1,823 ext. citations	4.4 avg, IF	5.45 L-index

#	Paper	IF	Citations
66	Stress–Strain Relations and Deformation Mechanisms of ZrN and HfN Superconductors. *Crystal Growth and Design*, **2022**, 22, 1104-1109	3.5	
65	Structural evolution and phase transition mechanism of [Formula: see text] under high pressure. *Scientific Reports*, **2021**, 11, 22090	4.9	
64	Indentation Strengths of Zirconium Diboride: Intrinsic versus Extrinsic Mechanisms. *Journal of Physical Chemistry Letters*, **2021**, 12, 2848-2853	6.4	32
63	Insights into the Structures and Bonding of Medium-Sized Cerium-Doped Boron Clusters. *Journal of Physical Chemistry A*, **2021**, 125, 4126-4132	2.8	3
62	Insights into the Bond Behavior and Mechanical Properties of Hafnium Carbide under High Pressure and High Temperature. *Inorganic Chemistry*, **2021**, 60, 515-524	5.1	6
61	Pressure-Driven Structural Phase Transitions and Superconductivity of Ternary Hydride MgVH6. *Journal of Physical Chemistry C*, **2021**, 125, 3150-3156	3.8	2
60	Phase stability and superconductivity of lead hydrides at high pressure. *Physical Review B*, **2021**, 103,	3.3	26
59	Identification of octahedral coordinated ZrN cationic clusters by mass spectrometry and structure searches. *Dalton Transactions*, **2021**, 50, 10187-10192	4.3	1
58	Two-Dimensional FeN Nanosheets: Ferromagnets and Nitrogen Diffusion. *Journal of Physical Chemistry Letters*, **2021**, 12, 8453-8459	6.4	2
57	Ternary Mg-Nb-H polyhydrides under high pressure. *Physical Review B*, **2021**, 104,	3.3	2
56	Structures, Mobilities, and Electronic Properties of Functionalized Silicene: Superhalogen BO Adsorption. *Inorganic Chemistry*, **2020**, 59, 5041-5049	5.1	8
55	LiB: A New Member of Tetrahedral-Typed B Ligand Half-Surround Cluster. *Scientific Reports*, **2020**, 10, 1642	4.9	9
54	Mechanical properties of tantalum carbide from high-pressure/high-temperature synthesis and first-principles calculations. *Physical Chemistry Chemical Physics*, **2020**, 22, 5018-5023	3.6	7
53	Modification of Geometric and Electronic Structures of Iron Clusters by Nitrogen: Fe8 vs Fe8N *Journal of Physical Chemistry C*, **2020**, 124, 3867-3872	3.8	7
52	Indentation-strain stiffening in tungsten nitrides: Mechanisms and implications. *Physical Review Materials*, **2020**, 4,	3.2	35
51	Structure-strength relations of distinct MoN phases from first-principles calculations. *Physical Review Materials*, **2020**, 4,	3.2	36
50	Exploring Physical Properties of Tantalum Carbide at High Pressure and Temperature. *Inorganic Chemistry*, **2020**, 59, 1848-1852	5.1	5

49	Tuning of Structure Evolution and Electronic Properties through Palladium-Doped Boron Clusters: PdB as a Motif for Boron-Based Nanotubes. *Journal of Physical Chemistry A*, **2020**, 124, 9187-9193	2.8	6
48	Elucidating Stress-Strain Relations of ZrB from First-Principles Studies. *Journal of Physical Chemistry Letters*, **2020**, 11, 9165-9170	6.4	50
47	Second group of high-pressure high-temperature lanthanide polyhydride superconductors. *Physical Review B*, **2020**, 102,	3.3	62
46	Negative Poisson Ratio in Two-Dimensional Tungsten Nitride: Synergistic Effect from Electronic and Structural Properties. *Journal of Physical Chemistry Letters*, **2020**, 11, 9643-9648	6.4	18
45	Probing the structural, bonding, electronic and magnetic properties of transition metal borazine systems: Com(borazine)n (m = 1, 2; n = 1 3). *Molecular Physics*, **2020**, 118, e1667542	1.7	1
44	Probing the structures, electronic and bonding properties of multidecker lanthanides: Neutral and anionic Ln(COT) (Ln = Ce, Nd, Eu, Ho and Yb; n, m = 1, 2) complexes. *Journal of Molecular Graphics and Modelling*, **2019**, 90, 226-234	2.8	3
43	New Theoretical Insights into the Crystal-Field Splitting and Transition Mechanism for Nd-Doped YAlO. *ACS Applied Materials & Interfaces*, **2019**, 11, 10745-10750	9.5	17
42	Probing the structure and electronic properties of beryllium doped boron clusters: A planar BeB cluster motif for metallo-borophene. *Scientific Reports*, **2019**, 9, 14367	4.9	16
41	Structural and Electronic Properties of Medium-Sized Aluminum-Doped Boron Clusters AlBn and Their Anions. *Journal of Physical Chemistry C*, **2019**, 123, 6276-6283	3.8	42
40	Abnormal physical behaviors of hafnium diboride under high pressure. *Applied Physics Letters*, **2019**, 115, 231903	3.4	8
39	Deciphering the Microstructure and Energy-Level Splitting of Tm-Doped Yttrium Aluminum Garnet. *Inorganic Chemistry*, **2019**, 58, 1058-1066	5.1	17
38	Geometric Structures and Electronic Properties of AlnV0/ (n = 5 14) Clusters: Photoelectron Spectroscopy and Theoretical Calculations. *Journal of Physical Chemistry C*, **2019**, 123, 1931-1938	3.8	8
37	Probing the Structural and Electronic Properties of Dirhenium Halide Clusters: A Density Functional Theory Study. *Scientific Reports*, **2018**, 8, 6702	4.9	3
36	Probing the Structural Evolution and Stabilities of Medium-Sized MoBn0/ Clusters. *Journal of Physical Chemistry C*, **2018**, 122, 20000-20005	3.8	32
35	Structural Stability and Evolution of Medium-Sized Tantalum-Doped Boron Clusters: A Half-Sandwich-Structured TaB Cluster. *Inorganic Chemistry*, **2018**, 57, 343-350	5.1	96
34	Structure and luminescence properties of a Nd3+ doped Bi4Ge3O12 scintillation crystal: new insights from a comprehensive study. *Journal of Materials Chemistry C*, **2017**, 5, 3079-3087	7.1	19
33	Evolution of the Structural and Electronic Properties of Medium-Sized Sodium Clusters: A Honeycomb-Like Na Cluster. *Inorganic Chemistry*, **2017**, 56, 1241-1248	5.1	63
32	Theoretical investigation of the electronic structure and luminescence properties for NdxY1 Al3(BO3)4 nonlinear laser crystal. *Journal of Materials Chemistry C*, **2017**, 5, 7174-7181	7.1	24

31	Iron-based magnetic superhalogens with pseudohalogens as ligands: An unbiased structure search. *Scientific Reports*, **2017**, 7, 45149	4.9	11
30	New insight into the structural evolution of PbTiO: an unbiased structure search. *Physical Chemistry Chemical Physics*, **2017**, 19, 1420-1424	3.6	3
29	A detailed investigation into the geometric and electronic structures of CoBQn (n = 2□10, Q = 0, □1) clusters. *New Journal of Chemistry*, **2017**, 41, 11208-11214	3.6	12
28	Prediction of Novel High-Pressure Structures of Magnesium Niobium Dihydride. *ACS Applied Materials & Interfaces*, **2017**, 9, 26169-26176	9.5	13
27	Structure and Electronic Properties of Neutral and Negatively Charged RhB Clusters (n = 3-10): A Density Functional Theory Study. *Journal of Physical Chemistry A*, **2017**, 121, 6510-6516	2.8	19
26	Prediction of the Iron-Based Polynuclear Magnetic Superhalogens with Pseudohalogen CN as Ligands. *Inorganic Chemistry*, **2017**, 56, 7928-7935	5.1	11
25	Theoretical investigation on the geometries and electronic properties of cesium□ilicon CsSi n (n = 2□12) clusters. *Structural Chemistry*, **2016**, 27, 457-465	1.8	2
24	Probing the low-energy structures of aluminum-magnesium alloy clusters: a detailed study. *Physical Chemistry Chemical Physics*, **2016**, 18, 26177-26183	3.6	39
23	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, 23296-303	3.6	3
22	Crystal Structures, Stabilities, Electronic Properties, and Hardness of MoB2: First-Principles Calculations. *Inorganic Chemistry*, **2016**, 55, 7033-40	5.1	30
21	Structural Evolutions and Crystal Field Characterizations of Tm-Doped YAlO: New Theoretical Insights. *ACS Applied Materials & Interfaces*, **2016**, 8, 30422-30429	9.5	27
20	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	7.1	15
19	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	3.8	78
18	First-principles study on the geometries, stabilities and electronic properties of yttrium□ilicon clusters (Y2Si n ; 1 □n □12). *Structural Chemistry*, **2016**, 27, 983-992	1.8	6
17	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	7.1	33
16	Insights into the geometries, electronic and magnetic properties of neutral and charged palladium clusters. *Scientific Reports*, **2016**, 6, 19656	4.9	62
15	Probing the structural evolution of ruthenium doped germanium clusters: Photoelectron spectroscopy and density functional theory calculations. *Scientific Reports*, **2016**, 6, 30116	4.9	34
14	Deciphering the Structural Evolution and Electronic Properties of Magnesium Clusters: An Aromatic Homonuclear Metal Mg Cluster. *Journal of Physical Chemistry A*, **2016**, 120, 7947-7954	2.8	53

13	Dynamical behavior of boron clusters. *Nanoscale*, **2016**, 8, 17639-17644	7.7	55
12	Structures, Stabilities, and Electronic Properties of Small-Sized Zr2Sin (n=1□11) Clusters: A Density Functional Study. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **2015**, 70, 805-814	1.4	3
11	Systematic theoretical investigation of structures, stabilities, and electronic properties of rhodium-doped silicon clusters: Rh2Si q n (n = 1□10; q = 0, □1). *Journal of Materials Science*, **2015**, 50, 6180-6196	4.3	9
10	Structures and bonding of auropolyboroenes [Au2(B4)xB3]□[Au2(B4)xB2]2□and [Au2(B4)xB]+ (x = 2, 3): comparison with dihydride polyboroenes. *RSC Advances*, **2015**, 5, 87855-87863	3.7	2
9	Prediction of Stable Ruthenium Silicides from First-Principles Calculations: Stoichiometries, Crystal Structures, and Physical Properties. *ACS Applied Materials & Interfaces*, **2015**, 7, 26776-82	9.5	35
8	Systematic theoretical investigation of geometries, stabilities and magnetic properties of iron oxide clusters (FeO)n□(n = 1□8, □= 0, □1): insights and perspectives. *RSC Advances*, **2015**, 5, 6560-6570	3.7	64
7	Understanding the structural transformation, stability of medium-sized neutral and charged silicon clusters. *Scientific Reports*, **2015**, 5, 15951	4.9	42
6	Exploration of stable stoichiometries, physical properties and hardness in the Rh□Si system: a first-principles study. *RSC Advances*, **2015**, 5, 53497-53503	3.7	8
5	Ab Initio Search for Global Minimum Structures of Pure and Boron Doped Silver Clusters. *Journal of Physical Chemistry A*, **2015**, 119, 6738-45	2.8	56
4	Theoretical study of the structures, stabilities, and electronic properties of neutral and anionic Ca2Si □ (n = 1□8, □= 0, +1) clusters. *European Physical Journal D*, **2014**, 68, 1	1.3	2
3	Hardness of FeB4: density functional theory investigation. *Journal of Chemical Physics*, **2014**, 140, 174505	3.9	67
2	Structural, Stabilities, and Electronic Properties of Bimetallic Mg2-doped Silicon Clusters. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **2014**, 69, 481-488	1.4	3
1	Theoretical investigation on the structural and thermodynamic properties of FeSe at high pressure and high temperature. *Dalton Transactions*, **2012**, 41, 9781-8	4.3	6