Xiao-yu Kuang

List of Publications by Year
in descending order

110 papers	2,010 citations	257101 24 h-index	276539 41 g-index
112 all docs	112 docs citations	112 times ranked	1406 citing authors

#	Article	IF	Citations
1	Spin-orbit coupling effect on pressure-induced phase transitions, magnetic, and electronic properties in YFeO3: A first-principles study. Chemical Physics, 2022, 555, 111454.	0.9	1
2	Structural Phase Transitions and Quantum Dots Regulation of Perovskite Stannates. Journal of Physical Chemistry C, 2022, 126, 4132-4139.	1.5	2
3	Tuning magnetic Mie-exciton interaction from the intermediate to strong coupling regime in a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">WSe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> monolayer coupled with dielectric-metal nanoresonators. Physical Review B, 2022, 105, .	1.1	12
4	Dissociation of dinitrogen on iron clusters: a detailed study of the Fe₁₆ + N₂ case. Physical Chemistry Chemical Physics, 2021, 23, 2166-2178.	1.3	6
5	Phase stability and superconductivity of lead hydrides at high pressure. Physical Review B, 2021, 103, .	1.1	60
6	Pressure-induced reconstructive phase transitions, polarization with metallicity, and enhanced hardness in antiperovskite MgCNi3. Physical Chemistry Chemical Physics, 2021, 23, 18221-18226.	1.3	1
7	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
8	Spectroscopic study of gap-surface plasmons in a metallic convex groove array and their applications in nanofocusing and plasmonic sensing. Physical Review B, 2021, 103, .	1.1	4
9	Single-Layer MX₂ (M = Zn, Cd and X = Cl, I): Auxetic Semiconductors with Strain-Tunable Optoelectronic Properties. Journal of Physical Chemistry C, 2021, 125, 12983-12990.	1.5	9
10	Two-Dimensional Fe₈N Nanosheets: Ferromagnets and Nitrogen Diffusion. Journal of Physical Chemistry Letters, 2021, 12, 8453-8459.	2.1	7
11	Pressure-Induced High-Î° Dielectric Properties and Multiple Phase Transitions between Novel Nonperovskite and Perovskite Phases in LiSbO3: A First-Principles Study. Journal of Physical Chemistry C, 2021, 125, 878-885.	1.5	2
12	Ternary Mg-Nb-H polyhydrides under high pressure. Physical Review B, 2021, 104, .	1.1	23
13	Coherent and incoherent coupling dynamics in a two-dimensional atomic crystal embedded in a plasmon-induced magnetic resonator. Physical Review B, 2020, 101, .	1.1	20
14	Investigation of the Structure and Luminescence Mechanism of Tm³⁺-Doped LiYF₄: New Theoretical Perspectives. Inorganic Chemistry, 2020, 59, 1211-1217.	1.9	11
15	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
16	Second group of high-pressure high-temperature lanthanide polyhydride superconductors. Physical Review B, 2020, 102, .	1.1	116
17	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
18	Semiconductor-to-metal reconstructive phase transition and superconductivity of anti-perovskite Ca3PN under hydrostatic pressure. Journal of Materials Chemistry C, 2020, 8, 13072-13078.	2.7	6

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19	LiB13: A New Member of Tetrahedral-Typed B13 Ligand Half-Surround Cluster. Scientific Reports, 2020, 10, 1642.	1.6	14
20	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
21	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
22	Strain-induced structural phase transition, electric polarization and unusual electric properties in photovoltaic materials CsMI3 (M = Pb, Sn). RSC Advances, 2020, 10, 12432-12438.	1.7	7
23	Structural evolution and electronic properties of medium-sized boron clusters doped with scandium. Journal of Physics Condensed Matter, 2019, 31, 485302.	0.7	18
24	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
25	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
26	Hydrostatic pressure induced structural phase transition and mechanical properties of fluoroperovskite. Journal of Physics Condensed Matter, 2019, 31, 505406.	0.7	7
27	Study of the Geometric Structures, Electronic and Magnetic Properties of Aluminium-Antimony Alloy Clusters. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2019, 74, 109-120.	0.7	1
28	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
29	Structural phases arising from reconstructive and isostructural transitions in high-melting-point oxides under hydrostatic pressure: A first-principles study. Physical Review B, 2018, 97, .	1.1	19
30	Probing the Structural and Electronic Properties of Dirhenium Halide Clusters: A Density Functional Theory Study. Scientific Reports, 2018, 8, 6702.	1.6	4
31	Insights into the Microstructure and Transition Mechanism for Nd³⁺-Doped Bi₄Si₃O₁₂: A Promising Near-Infrared Laser Material. Inorganic Chemistry, 2018, 57, 4563-4570.	1.9	11
32	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
33	Insights into the effects produced by doping of medium-sized boron clusters with ruthenium. Physical Chemistry Chemical Physics, 2018, 20, 30376-30383.	1.3	39
34	Probing the structural and electronic properties of zirconium doped boron clusters: Zr distorted B₁₂ ligand framework. Physical Chemistry Chemical Physics, 2018, 20, 23740-23746.	1.3	43
35	Novel type of ferroelectricity in brownmillerite structures: A first-principles study. Physical Review Materials, 2018, 2, .	0.9	8
36	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

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37	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
38	Ground State Properties of the Polar Alkali-Metalâ€“Ytterbium and Alkaline-Earth-Metalâ€“Ytterbium Molecules: A Comparative Study. Journal of Physical Chemistry A, 2017, 121, 2187-2193.	1.1	10
39	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
40	Probing the Interactions of O₂ with Small Gold Cluster Au_n^Q (n = 2â€“10, Q = 0, â^'1): A Neutral Chemisorbed Complex Au₅O₂ Cluster Predicted. Journal of Physical Chemistry C, 2017, 121, 24886-24893.	1.5	24
41	A systematic investigation of the geometries, electronic and magnetic properties of Al_nAs^q (q = â^'1, 0, +1; n = 1â€“16) clusters: a DFT calculation. Molecular Physics, 2017, 115, 3033-3043.	0.8	3
42	Prediction of Novel High-Pressure Structures of Magnesium Niobium Dihydride. ACS Applied Materials & Interfaces, 2017, 9, 26169-26176.	4.0	16
43	Exploration of the Structural, Electronic and Tunable Magnetic Properties of Cu4M (M = Sc-Ni) Clusters. Materials, 2017, 10, 946.	1.3	5
44	Insights into the geometries, electronic and magnetic properties of neutral and charged palladium clusters. Scientific Reports, 2016, 6, 19656.	1.6	73
45	Probing the structural evolution of ruthenium doped germanium clusters: Photoelectron spectroscopy and density functional theory calculations. Scientific Reports, 2016, 6, 30116.	1.6	45
46	Pressure effect on the properties of magnetic moments and phase transitions in YMnO₃ from first principles. RSC Advances, 2016, 6, 54041-54048.	1.7	6
47	Structural and Electronic Properties of Ruthenium-Doped Germanium Clusters. Journal of Physical Chemistry C, 2016, 120, 8399-8404.	1.5	39
48	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
49	Probing the low-energy structures of aluminumâ€“magnesium alloy clusters: a detailed study. Physical Chemistry Chemical Physics, 2016, 18, 26177-26183.	1.3	41
50	Dielectric properties of pyridineâ€“ethanol mixtures: density functional theory and experiments. RSC Advances, 2016, 6, 66007-66010.	1.7	8
51	High-temperature- and high-pressure-induced formation of the Laves-phase compoundXeS2. Physical Review B, 2016, 93, .	1.1	12
52	Structural Evolutions and Crystal Field Characterizations of Tm-Doped YAlO₃: New Theoretical Insights. ACS Applied Materials & Interfaces, 2016, 8, 30422-30429.	4.0	33
53	Large polarization and dielectric response in epitaxial SrZrO₃ films. Physical Chemistry Chemical Physics, 2016, 18, 7680-7687.	1.3	11
54	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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55	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
56	Understanding the structural transformation, stability of medium-sized neutral and charged silicon clusters. Scientific Reports, 2015, 5, 15951.	1.6	52
57	Structure, stability, and superconductivity of new Xeâ€“H compounds under high pressure. Journal of Chemical Physics, 2015, 143, 124310.	1.2	13
58	Theoretical study on the ground state of the polar alkali-metal-barium molecules: Potential energy curve and permanent dipole moment. Journal of Chemical Physics, 2015, 142, 034308.	1.2	9
59	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
60	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
61	Equation of State, Nonlinear Elastic Response, and Anharmonic Properties of Diamond-Cubic Silicon and Germanium: First-Principles Investigation. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2015, 70, 403-412.	0.7	4
62	Theoretical studies of the dependence of EPR parameters on local structure for the tetragonal Er3+ centres in YVO4 and ScVO4. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 150, 829-836.	2.0	5
63	Geometries, stabilities and fragmental channels of neutral and charged sulfur clusters: S_n^Q(n = 3â€“20, Q = 0, Â±1). Physical Chemistry Chemical Physics, 2015, 17, 13590-13597.	1.3	69
64	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
65	Comparing hydrostatic-pressure- and epitaxial-strain-induced phase transitions in multiferroic PbNiO3 from first principles. Solid State Communications, 2015, 203, 75-80.	0.9	11
66	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.	1.7	74
67	An ab initio study on the electronic and magnetic properties of MgO with intrinsic defects. RSC Advances, 2014, 4, 51366-51373.	1.7	24
68	Theoretical Search for an Ironâ€Based Magnetic Superhalogen with Halogen or Interhalogen as Ligand. European Journal of Inorganic Chemistry, 2014, 2014, 5885-5894.	1.0	2
69	A Systematic Investigation on Magnetism and Phase Stability of Cobalt. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2014, 69, 254-262.	0.7	2
70	Theoretical investigation on the structural phase transition, elastic properties and hardness of RhSi under high pressure. Journal of Alloys and Compounds, 2014, 592, 42-47.	2.8	13
71	Probing the structural and electronic properties of small aluminum dideuteride clusters. Journal of Molecular Graphics and Modelling, 2014, 53, 168-178.	1.3	3
72	DFT study of size-dependent geometries, stabilities and electronic properties of Si₂Ag_nclusters: comparison with pure silver clusters. Molecular Physics, 2014, 112, 972-981.	0.8	6

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73	Probing the structural and electronic properties of bimetallic Group-III metal-doped gold clusters: AunM2 (M = Na, Mg, Al; n = 1â€“8). European Physical Journal D, 2013, 67, 1.	0.6	12
74	Evolution of geometrical structures, stabilities and electronic properties of neutral and anionic LinCuÎ»(nâ€‰=â€‰1â€“9,Î»â€‰=â€‰0, â¯1) clusters: compare with pure lithium clusters. Molecular Physics, 2013, 111, 569-580.	0.8	7
75	Theoretical search for potential candidates as building blocks of hyperhalogens: BS2 and CrO4 molecules. RSC Advances, 2013, 3, 15449.	1.7	11
76	Effect of pressure on structural phase transition and elastic properties in NiSi. High Pressure Research, 2013, 33, 15-26.	0.4	4
77	Phase Stability, Physical Properties, and Hardness of Transition-Metal Diborides MB₂ (M =) Tj ETQq1 1 0.784314 rgBT /Ov	1.5	72
78	Investigation of the local structure and EPR spectra for Nd3+ in Bi4Ge3O12. Chemical Physics Letters, 2013, 557, 182-185.	1.2	7
79	A Systematic Search for Structures, Stabilities, Electronic and Magnetic Properties of Silicon Doped Silver Clusters: Comparison with Pure Silver Clusters. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2013, 68, 327-336.	0.7	0
80	Phase stability, mechanical properties, hardness, and possible reactive routing of chromium triboride from first-principle investigations. Journal of Chemical Physics, 2013, 139, 234503.	1.2	10
81	Investigation of Carbon Monoxide Adsorption on Cationic Gold- Palladium Clusters. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2013, 68, 651-658.	0.7	6
82	Structural and Electronic Properties of Stable AunIr2 (n = 1 â€“ 7) Clusters: Comparison with Pure Gold Clusters. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2012, 67, 729-738.	0.7	1
83	The defect structure and EPR parameters for Er3+in molybdates: a complete energy matrices study. Molecular Physics, 2012, 110, 3023-3029.	0.8	1
84	Density functional study of the structural and electronic properties of tetra-aluminum oxide (3â€‰â‰ˆâ€‰nâ€‰â‰ˆâ€‰8,â€‰Î»â€‰=â€‰0,â€‰â¯1) clusters. Molecular Physics, 2011, 109, 603-612.	0.8	10
85	Structural, electronic and magnetic properties of gold cluster doped with calcium: AunCa (nâ€‰=â€‰1â€“8). Molecular Physics, 2011, 109, 315-323.	0.8	16
86	Structural and electronic properties of silver-doped gold clusters Au_nAg^v(2â€‰â‰ˆâ€‰nâ€‰â‰ˆâ€‰10;vâ€‰=â€‰0,â€‰±1): comp pure gold clusters. Molecular Physics, 2011, 109, 2057-2068.		
87	Equilibrium Geometries, Stabilities, and Electronic Properties of the Bimetallic Ag₂-doped Si_n (n=1 â€“ 11) Clusters: A Density-Functional Investigation. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2011, 66, 353-362.	0.7	3
88	Optical and magnetic properties of transition-metal ions in tetrahedral and octahedral compounds. Science China: Physics, Mechanics and Astronomy, 2011, 54, 1796-1800.	2.0	6
89	Direct MP2 molecular dynamics studies of H atom reaction with CD₄ and CH₄. International Journal of Quantum Chemistry, 2011, 111, 4433-4442.	1.0	1
90	Theoretical Investigations of the Local Structure Distortion and EPR Parameter for Ni2+-doped Perovskite Fluorides. Chinese Journal of Chemical Physics, 2011, 24, 167-172.	0.6	1

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91	Comparative study of EPR spectra and crystal field effect on local structure for (NiF₆)^{4â^'}coordination complex in Ni²⁺:ZnF₂, NiF₂, and Ni²⁺:MgF₂systems. Physica Status Solidi (B): Basic Research, 2010, 247, 416-421.	0.7	5
92	Theoretical study of electron paramagnetic resonance spectra and local structure of trigonal [Cr(H2O)6]3+complex in GASH:Cr3+and AlCl3â€‰Â·â€‰6H2O:Cr3+systems at different temperatures. Physica Status Solidi (B): Basic Research, 2010, 247, 422-429.	0.7	0
93	Theoretical investigations of the local structure distortion and relationship between the EPR parameter and spin-orbit coupling coefficients for CsCdX₃:Ni²⁺(X = Cl, Br) systems. Molecular Physics, 2010, 108, 1899-1906.	0.8	3
94	Surface Magnetic Effects in an Alternating Superlattice. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2009, 64, 753-757.	0.7	0
95	Local Structure Determination of Tetragonal Cr²⁺ Center in CdS Semiconductor. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2009, 64, 507-510.	0.7	0
96	The Curie Temperature of the Ferroelectric Superlattice Films with Surface Modification. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2009, 64, 723-728.	0.7	0
97	Structural, spectral characterization and electron paramagnetic resonance studies of Ni²⁺ions in various compounds: KZnF₃, CdCl₂, CdBr₂and CsMgI₃. Molecular Physics, 2009, 107, 133-141.	0.8	7
98	EPR and optical spectra of Ni2+-VAgin silver chloride and silver bromide. Molecular Physics, 2009, 107, 621-627.	0.8	2
99	Effects of Concentration, Temperature and Hydrostatic Pressure on the Local Lattice Structure of Ni2+ Doped Zn(BF4)2 Â· 6H2O Crystal. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2009, 64, 511-517.	0.7	1
100	Effect on the EPR and local lattice structure distortion of V3+ion doping corundum crystal: three models studied. Molecular Physics, 2008, 106, 1879-1885.	0.8	1
101	Local defect structures and EPR studies on (FeO6)9- and (FeO4)5- clusters in YGG: Fe3+ system. Molecular Physics, 2008, 106, 2643-2648.	0.8	0
102	Theoretical study of the dependence of EPR spectra on local structure for octahedral Cr3+centres in oxides and fluorides series. Molecular Physics, 2008, 106, 999-1006.	0.8	7
103	Theoretical study of spin-singlet contributions to zero-field splitting of a 3d⁶ion in a trigonal ligand field and applications to Fe²⁺in FeSiF₆Â· 6H₂O and FeCO₃. Molecular Physics, 2008, 106, 2677-2683.	0.8	1
104	Investigation of local lattice structure around Cr³⁺ions at the trigonal and tetragonal sites in RbCdF₃: Cr³⁺crystal. Molecular Physics, 2008, 106, 1033-1038.	0.8	1
105	Phase Transition Properties of a Ferroelectric Superlattice with Surface Modification. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2008, 63, 351-358.	0.7	0
106	Investigation of the Local Lattice Structure and the Effects of the Orbital Reduction Factor on the g Factors of a Trigonal [Ni(H2O)6]2+ Cluster in NiTiF6 Â· 6H2O and ZnSiF6 Â· 6H2O Crystals at Different Temperatures. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2008, 63, 609-615.	0.7	1
107	Theoretical study of local lattice structure of (FeOF5)4â^'cluster in diamagnetic pervoskite RbCdF3. Molecular Physics, 2008, 106, 723-728.	0.8	0
108	Homotrinuclear Spin Cluster with Orbital Degeneracy in a Magnetic Field: Algebraic Dynamic Studies of the Geometric Phase January 25, 2008. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2008, 63, 405-411.	0.7	0

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109	EPR Theoretical Study of the Local Lattice Structure of Fe3+ Doped in MgTiO3 and LiTaO3. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2007, 62, 101-106.	0.7	0
110	The Local Structure Distortion of Chromium-Phosphorus Clusters as Cr²⁺ Impurity in InP Semiconductors. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2006, 61, 371-374.	0.7	0