Xiaoyu Kuang

List of Publications by Year in descending order

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41 papers	762 citations	471061 17 h-index	552369 26 g-index
41 all docs	41 docs citations	41 times ranked	650 citing authors

#	Article	IF	Citations
1	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
2	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
3	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
4	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
5	Probing the low-energy structures of aluminumâ€“magnesium alloy clusters: a detailed study. Physical Chemistry Chemical Physics, 2016, 18, 26177-26183.	1.3	41
6	Structural and Electronic Properties of Ruthenium-Doped Germanium Clusters. Journal of Physical Chemistry C, 2016, 120, 8399-8404.	1.5	39
7	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
8	Structural Evolutions and Crystal Field Characterizations of Tm-Doped YAlO₃: New Theoretical Insights. ACS Applied Materials & Interfaces, 2016, 8, 30422-30429.	4.0	33
9	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
10	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
11	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
12	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
13	Deciphering the Microstructure and Energy-Level Splitting of Tm³⁺-Doped Yttrium Aluminum Garnet. Inorganic Chemistry, 2019, 58, 1058-1066.	1.9	23
14	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
15	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
16	Structural evolution and electronic properties of medium-sized boron clusters doped with scandium. Journal of Physics Condensed Matter, 2019, 31, 485302.	0.7	18
17	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
18	In-Depth Determination of the Microstructure and Energy Transition Mechanism for Nd³⁺-Doped Yttrium Oxide Laser Crystals. Journal of Physical Chemistry C, 2020, 124, 2113-2119.	1.5	16

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19	Local structure and EPR g factors for KAl(MoO4)2:Cr3+ and RbIn(MoO4)2:Cr3+ systems. Journal of Alloys and Compounds, 2008, 448, 6-10.	2.8	11
20	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
21	Large polarization and dielectric response in epitaxial SrZrO₃ films. Physical Chemistry Chemical Physics, 2016, 18, 7680-7687.	1.3	11
22	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
23	First-principle study of the microstructure and electronic properties for Cr3+ doped yttrium orthoaluminate. Computational Materials Science, 2020, 174, 109467.	1.4	11
24	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
25	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
26	Novel structural phases and the electrical properties of Si3B under high pressure. Physical Chemistry Chemical Physics, 2017, 19, 16206-16212.	1.3	9
27	Prediction of hypervalent molecules: investigation on M_nC (M = Li, Na, K, Rb and Cs; n =) Tj ETQq1 1 0.784314 rgBT /Ove	1.3	9
28	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
29	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
30	Novel type of ferroelectricity in brownmillerite structures: A first-principles study. Physical Review Materials, 2018, 2, .	0.9	8
31	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
32	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
33	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
34	Insights into the Microstructures and Energy Levels of Pr³⁺-Doped YAlO₃ Scintillating Crystals. Inorganic Chemistry, 2021, 60, 5107-5113.	1.9	6
35	Deciphering the structures and electronic features of Yb3+-doped Y2O3 crystal: A theoretical perspective study. Computational Materials Science, 2021, 192, 110340.	1.4	6
36	Semi-empirical calculations of radiative rates for parity-forbidden transitions within the 4f2configuration of Ba-like ions La+, Ce2+, Pr3+and Nd4+and 4f12configuration of Dy-like Yb4+. Journal of Physics B: Atomic, Molecular and Optical Physics, 2014, 47, 145002.	0.6	5

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37	The Microstructure and Electronic Properties of Yttrium Oxide Doped With Cerium: A Theoretical Insight. Frontiers in Chemistry, 2020, 8, 338.	1.8	5
38	Exploration of the novel structures and electronic properties for Nd3+ doped CaTiO3. Materials Chemistry and Physics, 2021, 266, 124525.	2.0	2
39	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
40	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
41	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