# Xiaoyu Kuang

## List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/7282499/publications.pdf

Version: 2024-02-01

| | | | |
|---|---|---|---|
| 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 | 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 | Dissociation of dinitrogen on iron clusters: a detailed study of the Fe<sub>16</sub> + N<sub>2</sub> case. Physical Chemistry Chemical Physics, 2021, 23, 2166-2178. | 1.3 | 6 |
| 3 | 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 |
| 4 | Insights into the Microstructures and Energy Levels of Pr<sup>3+</sup>-Doped YAlO<sub>3</sub> Scintillating Crystals. Inorganic Chemistry, 2021, 60, 5107-5113. | 1.9 | 6 |
| 5 | Deciphering the structures and electronic features of Yb3+-doped Y2O3 crystal: A theoretical perspective study. Computational Materials Science, 2021, 192, 110340. | 1.4 | 6 |
| 6 | 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 |
| 7 | Single-Layer MX<sub>2</sub> (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 |
| 8 | Exploration of the novel structures and electronic properties for Nd3+ doped CaTiO3. Materials Chemistry and Physics, 2021, 266, 124525. | 2.0 | 2 |
| 9 | First-principle study of the microstructure and electronic properties for Cr3+ doped yttrium orthoaluminate. Computational Materials Science, 2020, 174, 109467. | 1.4 | 11 |
| 10 | In-Depth Determination of the Microstructure and Energy Transition Mechanism for Nd<sup>3+</sup>-Doped Yttrium Oxide Laser Crystals. Journal of Physical Chemistry C, 2020, 124, 2113-2119. | 1.5 | 16 |
| 11 | Tuning of Structure Evolution and Electronic Properties through Palladium-Doped Boron Clusters: PdB<sub>16</sub> as a Motif for Boron-Based Nanotubes. Journal of Physical Chemistry A, 2020, 124, 9187-9193. | 1.1 | 11 |
| 12 | 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 |
| 13 | The Microstructure and Electronic Properties of Yttrium Oxide Doped With Cerium: A Theoretical Insight. Frontiers in Chemistry, 2020, 8, 338. | 1.8 | 5 |
| 14 | 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 |
| 15 | 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 |
| 16 | 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 |
| 17 | Structural evolution and electronic properties of medium-sized boron clusters doped with scandium. Journal of Physics Condensed Matter, 2019, 31, 485302. | 0.7 | 18 |
| 18 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | New Theoretical Insights into the Crystal-Field Splitting and Transition Mechanism for Nd<sup>3+</sup>-Doped Y<sub>3</sub>Al<sub>5</sub>O<sub>12</sub>. ACS Applied Materials & Interfaces, 2019, 11, 10745-10750. | 4.0 | 22 |
| 20 | Structural and Electronic Properties of Medium-Sized Aluminum-Doped Boron Clusters AlB<sub>n</sub> and Their Anions. Journal of Physical Chemistry C, 2019, 123, 6276-6283. | 1.5 | 59 |
| 21 | Deciphering the Microstructure and Energy-Level Splitting of Tm<sup>3+</sup>-Doped Yttrium Aluminum Garnet. Inorganic Chemistry, 2019, 58, 1058-1066. | 1.9 | 23 |
| 22 | 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 |
| 23 | 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 |
| 24 | Insights into the Microstructure and Transition Mechanism for Nd<sup>3+</sup>-Doped Bi<sub>4</sub>Si<sub>3</sub>O<sub>12</sub>: A Promising Near-Infrared Laser Material. Inorganic Chemistry, 2018, 57, 4563-4570. | 1.9 | 11 |
| 25 | 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 |
| 26 | Probing the structural and electronic properties of zirconium doped boron clusters: Zr distorted B<sub>12</sub> ligand framework. Physical Chemistry Chemical Physics, 2018, 20, 23740-23746. | 1.3 | 43 |
| 27 | Novel type of ferroelectricity in brownmillerite structures: A first-principles study. Physical Review Materials, 2018, 2, . | 0.9 | 8 |
| 28 | Structure and luminescence properties of a Nd<sup>3+</sup>doped Bi<sub>4</sub>Ge<sub>3</sub>O<sub>12</sub>scintillation crystal: new insights from a comprehensive study. Journal of Materials Chemistry C, 2017, 5, 3079-3087. | 2.7 | 27 |
| 29 | Novel structural phases and the electrical properties of Si3B under high pressure. Physical Chemistry Chemical Physics, 2017, 19, 16206-16212. | 1.3 | 9 |
| 30 | Theoretical investigation of the electronic structure and luminescence properties for Nd<sub>x</sub>Y<sub>1â^'x</sub>Al<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>nonlinear laser crystal. Journal of Materials Chemistry C, 2017, 5, 7174-7181. | 2.7 | 30 |
| 31 | Prediction of hypervalent molecules: investigation on M<sub>n</sub>C (M = Li, Na, K, Rb and Cs; n =) Tj ETQq1 1 0.784314 rgBT /Overl | 1.3 | 9 |
| 32 | Structural and Electronic Properties of Ruthenium-Doped Germanium Clusters. Journal of Physical Chemistry C, 2016, 120, 8399-8404. | 1.5 | 39 |
| 33 | Probing the low-energy structures of aluminumâ€“magnesium alloy clusters: a detailed study. Physical Chemistry Chemical Physics, 2016, 18, 26177-26183. | 1.3 | 41 |
| 34 | Structural Evolutions and Crystal Field Characterizations of Tm-Doped YAlO<sub>3</sub>: New Theoretical Insights. ACS Applied Materials & Interfaces, 2016, 8, 30422-30429. | 4.0 | 33 |
| 35 | Large polarization and dielectric response in epitaxial SrZrO<sub>3</sub> films. Physical Chemistry Chemical Physics, 2016, 18, 7680-7687. | 1.3 | 11 |
| 36 | Determination of the microstructure, energy levels and magnetic dipole transition mechanism for Tm<sup>3+</sup>doped yttrium aluminum borate. Journal of Materials Chemistry C, 2016, 4, 1988-1995. | 2.7 | 17 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | 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 |
| 38 | 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 |
| 39 | Systematic theoretical investigation of geometries, stabilities and magnetic properties of iron oxide clusters (FeO)‹sub›n‹/sub›‹sup›Î¼‹/sup›(n = 1â€“8, Î¼ = 0, Â±1): insights and perspectives. RSC Advances, 2015, 5, 6560-6570. | 3.1 | 74 |
| 40 | 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 |
| 41 | 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 |