

# Xiao-Yong Yang

## List of Publications by Year in descending order

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37  
papers

884  
citations

471061

17  
h-index

476904

29  
g-index

37  
all docs

37  
docs citations

37  
times ranked

610  
citing authors

#	ARTICLE	IF	CITATIONS
1	Metal-free 2D/2D C <sub>3</sub> N <sub>5</sub> /GO nanosheets with customized energy-level structure for radioactive nuclear wastewater treatment. <i>Journal of Hazardous Materials</i> , 2022, 422, 126912.	6.5	49
2	Three-dimensional C <sub>3</sub> N <sub>5</sub> /RGO aerogels with enhanced visible-light response and electron-hole separation efficiency for photocatalytic uranium reduction. <i>Chemical Engineering Journal</i> , 2022, 427, 131773.	6.6	56
3	Machine learning-enabled band gap prediction of monolayer transition metal chalcogenide alloys. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 4653-4665.	1.3	7
4	Synergistic Effect of the Sulfur Vacancy and Schottky Heterojunction on Photocatalytic Uranium Immobilization: The Thermodynamics and Kinetics. <i>Inorganic Chemistry</i> , 2022, 61, 2242-2250.	1.9	22
5	Structural stability and aqueous durability of Cs incorporation into BaAl <sub>2</sub> Ti <sub>6</sub> O <sub>16</sub> hollandite. <i>Journal of Nuclear Materials</i> , 2022, 565, 153716.	1.3	4
6	Interface Engineering of Co(OH) <sub>2</sub> Nanosheets Growing on the KNbO <sub>3</sub> Perovskite Based on Electronic Structure Modulation for Enhanced Peroxymonosulfate Activation. <i>Environmental Science &amp; Technology</i> , 2022, 56, 5200-5212.	4.6	136
7	Structural, electronic, mechanical and thermodynamic properties of U <sup>4+</sup> -Si intermetallic compounds: A comprehensive first principles calculations. <i>Progress in Nuclear Energy</i> , 2022, 148, 104229.	1.3	5
8	Exploring Janus MoSSe monolayer as a workable media for SOF <sub>6</sub> decompositions sensing based on DFT calculations. <i>Computational Materials Science</i> , 2021, 186, 109976.	1.4	21
9	Defect evolution behaviors from single sulfur point vacancies to line vacancies in monolayer molybdenum disulfide. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19525-19536.	1.3	6
10	Synergistic vacancy defects and mechanical strain for the modulation of the mechanical, electronic and optical properties of monolayer tungsten disulfide. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6298-6308.	1.3	5
11	What is the Role of Nb on Preferential Hydriding of Double-Phased Uranium, Stabilizing <sup>135</sup> U, or Avoiding Hydrogen Aggregation?. <i>Journal of Physical Chemistry C</i> , 2021, 125, 9364-9370.	1.5	0
12	Rapid preparation of zirconia/zircon composites ceramics by microwave method: Experiment and first-principle investigation. <i>Progress in Nuclear Energy</i> , 2021, 139, 103839.	1.3	2
13	Enhanced overall water splitting under visible light of MoSSe/WSSe heterojunction by lateral interfacial engineering. <i>Journal of Catalysis</i> , 2021, 404, 18-31.	3.1	13
14	Efficient photoreduction strategy for uranium immobilization based on graphite carbon nitride/perovskite oxide heterojunction nanocomposites. <i>Applied Catalysis B: Environmental</i> , 2021, 298, 120625.	10.8	51
15	Recent Advancements and Future Prospects in Ultrathin 2D Semiconductor-Based Photocatalysts for Water Splitting. <i>Catalysts</i> , 2020, 10, 1111.	1.6	35
16	Exploring the Degradation Behavior of Ce-Monazite in Water Solution through Adsorption and Penetration Kinetics. <i>Journal of Physical Chemistry C</i> , 2020, 124, 22173-22184.	1.5	10
17	Revealing the Charge Storage Mechanism of Nickel Oxide Electrochromic Supercapacitors. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 39098-39107.	4.0	82
18	Unveiling the energetic and structural properties of Pu doped zircon through electrochemical equilibrium diagram from DFT+U calculations. <i>Journal of Nuclear Materials</i> , 2020, 539, 152234.	1.3	0

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19	Structural Insight of the Frailty of 2D Janus NbSeTe as an Active Photocatalyst. ChemCatChem, 2020, 12, 6013-6023.	1.8	20
20	Strain-Engineered Metal-Free h-B <sub>2</sub> O Monolayer as a Mechanocatalyst for Photocatalysis and Improved Hydrogen Evolution Reaction. Journal of Physical Chemistry C, 2020, 124, 7884-7892.	1.5	27
21	Fluoride ion batteries: Designing flexible M <sub>2</sub> CH <sub>2</sub> (M=Ti or V) MXenes as high-capacity cathode materials. Nano Energy, 2020, 74, 104911.	8.2	27
22	Sensing the polar molecules MH <sub>3</sub> (M = N, P, or As) with a Janus NbTeSe monolayer. New Journal of Chemistry, 2020, 44, 7932-7940.	1.4	20
23	Investigating the solution and diffusion properties of hydrogen in $\delta$ -Uranium by first-principles calculations. Progress in Nuclear Energy, 2020, 122, 103268.	1.3	8
24	Probing the active sites of newly predicted stable Janus scandium dichalcogenides for photocatalytic water-splitting. Catalysis Science and Technology, 2019, 9, 4981-4989.	2.1	28
25	Interfacial aspect of ZnTe/In <sub>2</sub> Te <sub>3</sub> heterostructures as an efficient catalyst for the hydrogen evolution reaction. Journal of Materials Chemistry A, 2019, 7, 27441-27449.	5.2	41
26	An emerging Janus MoSeTe material for potential applications in optoelectronic devices. Journal of Materials Chemistry C, 2019, 7, 12312-12320.	2.7	85
27	First-principles calculations and experiments for Ce <sup>4+</sup> effects on structure and chemical stabilities of Zr <sub>1</sub> -Ce SiO <sub>4</sub> . Journal of Nuclear Materials, 2019, 514, 276-283.	1.3	11
28	Effect of phase evolution and acidity on the chemical stability of Zr <sub>1</sub> -Nd SiO <sub>4</sub> /2 ceramics. Ceramics International, 2019, 45, 3052-3058.	2.3	10
29	First-principles investigation on stability and diffusion mechanism of helium impurities in 4H-SiC. Journal of Nuclear Materials, 2018, 499, 168-174.	1.3	6
30	Structures and energetics of point defects with charge states in zircon: A first-principles study. Journal of Alloys and Compounds, 2018, 759, 60-69.	2.8	4
31	First-principles GGA+ $\hat{U}$ calculation investigating the hydriding and diffusion properties of hydrogen in PuH <sub>2</sub> <sup>+</sup> , O $\hat{A}$ % $\hat{x}$ % $\hat{A}$ 1. International Journal of Hydrogen Energy, 2018, 43, 13632-13638.	3.8	17
32	First-principles study of hydrogen retention and diffusion behaviors in 4H-SiC. Superlattices and Microstructures, 2018, 122, 362-370.	1.4	1
33	First-principles study of the stability and diffusion properties of hydrogen in zirconium carbide. Journal of Nuclear Materials, 2016, 479, 130-136.	1.3	14
34	First-principles study of migration and diffusion mechanisms of helium in $\delta$ -Be. AIP Advances, 2016, 6, .	0.6	5
35	Mechanical, electronic, and thermodynamic properties of zirconium carbide from first-principles calculations. Chinese Physics B, 2015, 24, 116301.	0.7	17
36	First-principles study of native point defects and diffusion behaviors of helium in zirconium carbide. Journal of Nuclear Materials, 2015, 465, 161-166.	1.3	26

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37	The temperature-dependent diffusion coefficient of helium in zirconium carbide studied with first-principles calculations. Journal of Applied Physics, 2015, 117, .	1.1	13