

Xiao-Yong Yang

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Interface Engineering of Co(OH) ₂ Nanosheets Growing on the KNbO ₃ Perovskite Based on Electronic Structure Modulation for Enhanced Peroxymonosulfate Activation. Environmental Science & Technology, 2022, 56, 5200-5212.	10.0	136
2	An emerging Janus MoSeTe material for potential applications in optoelectronic devices. Journal of Materials Chemistry C, 2019, 7, 12312-12320.	5.5	85
3	Revealing the Charge Storage Mechanism of Nickel Oxide Electrochromic Supercapacitors. ACS Applied Materials & Interfaces, 2020, 12, 39098-39107.	8.0	82
4	Three-dimensional C3N5/RGO aerogels with enhanced visible-light response and electron-hole separation efficiency for photocatalytic uranium reduction. Chemical Engineering Journal, 2022, 427, 131773.	12.7	56
5	Efficient photoreduction strategy for uranium immobilization based on graphite carbon nitride/perovskite oxide heterojunction nanocomposites. Applied Catalysis B: Environmental, 2021, 298, 120625.	20.2	51
6	Metal-free 2D/2D C3N5/GO nanosheets with customized energy-level structure for radioactive nuclear wastewater treatment. Journal of Hazardous Materials, 2022, 422, 126912.	12.4	49
7	Interfacial aspect of ZnTe/In ₂ Te ₃ heterostructures as an efficient catalyst for the hydrogen evolution reaction. Journal of Materials Chemistry A, 2019, 7, 27441-27449.	10.3	41
8	Recent Advancements and Future Prospects in Ultrathin 2D Semiconductor-Based Photocatalysts for Water Splitting. Catalysts, 2020, 10, 1111.	3.5	35
9	Probing the active sites of newly predicted stable Janus scandium dichalcogenides for photocatalytic water-splitting. Catalysis Science and Technology, 2019, 9, 4981-4989.	4.1	28
10	Strain-Engineered Metal-Free h-B ₂ O Monolayer as a Mechanocatalyst for Photocatalysis and Improved Hydrogen Evolution Reaction. Journal of Physical Chemistry C, 2020, 124, 7884-7892.	3.1	27
11	Fluoride ion batteries: Designing flexible M2CH2 (M=Ti or V) MXenes as high-capacity cathode materials. Nano Energy, 2020, 74, 104911.	16.0	27
12	First-principles study of native point defects and diffusion behaviors of helium in zirconium carbide. Journal of Nuclear Materials, 2015, 465, 161-166.	2.7	26
13	Synergistic Effect of the Sulfur Vacancy and Schottky Heterojunction on Photocatalytic Uranium Immobilization: The Thermodynamics and Kinetics. Inorganic Chemistry, 2022, 61, 2242-2250.	4.0	22
14	Exploring Janus MoSSe monolayer as a workable media for SOF6 decompositions sensing based on DFT calculations. Computational Materials Science, 2021, 186, 109976.	3.0	21
15	Structural Insight of the Frailty of 2D Janus NbSeTe as an Active Photocatalyst. ChemCatChem, 2020, 12, 6013-6023.	3.7	20
16	Sensing the polar molecules MH3 (M = N, P, or As) with a Janus NbTeSe monolayer. New Journal of Chemistry, 2020, 44, 7932-7940.	2.8	20
17	Mechanical, electronic, and thermodynamic properties of zirconium carbide from first-principles calculations. Chinese Physics B, 2015, 24, 116301.	1.4	17
18	First-principles GGA+U calculation investigating the hydriding and diffusion properties of hydrogen in PuH2+, O ₂ . International Journal of Hydrogen Energy, 2018, 43, 13632-13638.	7.1	17

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19	First-principles study of the stability and diffusion properties of hydrogen in zirconium carbide. Journal of Nuclear Materials, 2016, 479, 130-136.	2.7	14
20	The temperature-dependent diffusion coefficient of helium in zirconium carbide studied with first-principles calculations. Journal of Applied Physics, 2015, 117, .	2.5	13
21	Enhanced overall water splitting under visible light of MoSSe \times WSSe heterojunction by lateral interfacial engineering. Journal of Catalysis, 2021, 404, 18-31.	6.2	13
22	First-principles calculations and experiments for Ce ⁴⁺ effects on structure and chemical stabilities of Zr ₁ -Ce SiO ₄ . Journal of Nuclear Materials, 2019, 514, 276-283.	2.7	11
23	Effect of phase evolution and acidity on the chemical stability of Zr ₁ -Nd SiO ₄ /2 ceramics. Ceramics International, 2019, 45, 3052-3058.	4.8	10
24	Exploring the Degradation Behavior of Ce-Monazite in Water Solution through Adsorption and Penetration Kinetics. Journal of Physical Chemistry C, 2020, 124, 22173-22184.	3.1	10
25	Investigating the solution and diffusion properties of hydrogen in δ -Uranium by first-principles calculations. Progress in Nuclear Energy, 2020, 122, 103268.	2.9	8
26	Machine learning-enabled band gap prediction of monolayer transition metal chalcogenide alloys. Physical Chemistry Chemical Physics, 2022, 24, 4653-4665.	2.8	7
27	First-principles investigation on stability and diffusion mechanism of helium impurities in 4H-SiC. Journal of Nuclear Materials, 2018, 499, 168-174.	2.7	6
28	Defect evolution behaviors from single sulfur point vacancies to line vacancies in monolayer molybdenum disulfide. Physical Chemistry Chemical Physics, 2021, 23, 19525-19536.	2.8	6
29	First-principles study of migration and diffusion mechanisms of helium in δ -Be. AIP Advances, 2016, 6, .	1.3	5
30	Synergistic vacancy defects and mechanical strain for the modulation of the mechanical, electronic and optical properties of monolayer tungsten disulfide. Physical Chemistry Chemical Physics, 2021, 23, 6298-6308.	2.8	5
31	Structural, electronic, mechanical and thermodynamic properties of U δ -Si intermetallic compounds: A comprehensive first principles calculations. Progress in Nuclear Energy, 2022, 148, 104229.	2.9	5
32	Structures and energetics of point defects with charge states in zircon: A first-principles study. Journal of Alloys and Compounds, 2018, 759, 60-69.	5.5	4
33	Structural stability and aqueous durability of Cs incorporation into BaAl ₂ Ti ₆ O ₁₆ hollandite. Journal of Nuclear Materials, 2022, 565, 153716.	2.7	4
34	Rapid preparation of zirconia/zircon composites ceramics by microwave method: Experiment and first-principle investigation. Progress in Nuclear Energy, 2021, 139, 103839.	2.9	2
35	First-principles study of hydrogen retention and diffusion behaviors in 4H-SiC. Superlattices and Microstructures, 2018, 122, 362-370.	3.1	1
36	Unveiling the energetic and structural properties of Pu doped zircon through electrochemical equilibrium diagram from DFT+U calculations. Journal of Nuclear Materials, 2020, 539, 152234.	2.7	0

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37	What is the Role of Nb on Preferential Hydriding of Double-Phased Uranium, Stabilizing $\delta^3\text{-U}$, or Avoiding Hydrogen Aggregation?. Journal of Physical Chemistry C, 2021, 125, 9364-9370.	3.1	0