Xiaoqiang Liu

List of Publications by Year in descending order

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69 papers	1,464 citations	331538 21 h-index	360920 35 g-index
69 all docs	69 docs citations	69 times ranked	2398 citing authors

#	Article	IF	Citations
1	Exploration of Metal-Molecule interaction of subnanometric heterogeneous catalysts via simulated Raman spectrum. Applied Surface Science, 2022, 579, 152194.	3.1	2
2	Detection and tuning of spin-orbit interactions on inclined-grown Bi2O2Se nanoplates. Applied Physics Letters, 2022, 120, .	1.5	7
3	Pressureâ€Induced Amorphization and Crystallization of Heterophase Pd Nanostructures. Small, 2022, 18, e2106396.	5.2	9
4	Silver(II) route to unconventional superconductivity. Physical Review B, 2022, 105, .	1.1	2
5	Unveiling the origin of alkali metal promotion in CO2 methanation over Ru/ZrO2. Applied Catalysis B: Environmental, 2022, 314, 121476.	10.8	27
6	Charge doping to flat AgF₂ monolayers in a chemical capacitor setup. Physical Chemistry Chemical Physics, 2022, 24, 15705-15717.	1.3	3
7	Structure and flow properties of coal ash slag using ring statistics and molecular dynamics simulation: Role of CaO/Na2O in SiO2â€“Al2O3â€“CaOâ€“Na2O. Chemical Engineering Science, 2021, 231, 116285.	1.9	19
8	Mesoporous RhRu Nanosponges with Enhanced Water Dissociation toward Efficient Alkaline Hydrogen Evolution. ACS Applied Materials & Interfaces, 2021, 13, 5052-5060.	4.0	30
9	Theoretical Perspectives on the Modulation of Carbon on Transition-Metal Catalysts for Conversion of Carbon-Containing Resources. ACS Catalysis, 2021, 11, 2156-2181.	5.5	34
10	Methanol electrooxidation on core-shell Ag@Pd catalysts. Electrochemistry Communications, 2021, 123, 106917.	2.3	15
11	Electrical Spin Injection into the 2D Electron Gas in AlN/GaN Heterostructures with Ultrathin AlN Tunnel Barrier. Advanced Functional Materials, 2021, 31, 2009771.	7.8	11
12	Carbon Deposition and Permeation on Nickel Surfaces in Operando Conditions: A Theoretical Study. Journal of Physical Chemistry C, 2021, 125, 7166-7177.	1.5	14
13	The role of ligands in pressure-induced phase transition of gold nanoribbons. Phase Transitions, 2021, 94, 123-133.	0.6	2
14	Spin dynamics in GaN/Al0.1Ga0.9N quantum well with complex band edge structure. Applied Physics Letters, 2021, 118, 252107.	1.5	4
15	Carbon nanoparticle coated by silicon dioxide supported platinum nanoparticles towards oxygen reduction reaction. Materials Research Bulletin, 2021, 139, 111268.	2.7	7
16	Why phenol is selectively hydrogenated to cyclohexanol on Ru (0001): An experimental and theoretical study. Applied Surface Science, 2021, 558, 149880.	3.1	16
17	Insights into Coke Formation and Removal under Operating Conditions with a Quantum Nanoreactor Approach. Journal of Physical Chemistry Letters, 2021, 12, 9413-9421.	2.1	4
18	Excitonic effects on electron spin orientation and relaxation in wurtzite GaN. Physical Review B, 2021, 104, .	1.1	3

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19	Oxygen Adsorption-Induced Morphological Evolution of HÃgg Iron Carbide at High Oxygen Chemical Potentials. Journal of Physical Chemistry C, 2021, 125, 3055-3065.	1.5	3
20	A combined DFTB nanoreactor and reaction network generator approach for the mechanism of hydrocarbon combustion. Chemical Communications, 2021, 57, 11633-11636.	2.2	6
21	Assembly of Silicalite-1 Crystals Like Toy Lego Bricks into One-, Two-, and Three-Dimensional Architectures for Enhancing Its Adsorptive Separation and Catalytic Performances. ACS Applied Materials & Interfaces, 2021, 13, 58085-58095.	4.0	5
22	Quantifying the photocatalytic role and activity at the edge and surface of Pd co-catalysts using N₂ fixation as a case. Journal of Materials Chemistry A, 2021, 9, 26036-26044.	5.2	5
23	C2 weakens the turnover frequency during the melting of Fe_xC_y: insights from reactive MD simulations. New Journal of Chemistry, 2021, 46, 282-293.	1.4	1
24	Temperature-dependent surface free energy and the Wulff shape of iron and iron carbide nanoparticles: A molecular dynamics study. Applied Surface Science, 2020, 509, 144859.	3.1	13
25	Theoretical exploration of intrinsic facet-dependent CH4 and C2 formation on Fe5C2 particle. Applied Catalysis B: Environmental, 2020, 278, 119308.	10.8	30
26	Theoretical Insights into the Structure and Activity of Cobalt Modulated by Surface and Subsurface Carbon in Operando Conditions. Journal of Physical Chemistry C, 2020, 124, 18576-18586.	1.5	5
27	In situ tuning of electronic structure of catalysts using controllable hydrogen spillover for enhanced selectivity. Nature Communications, 2020, 11, 4773.	5.8	81
28	The driving effect of substituent size changes on reaction: a novel reaction for direct production of triacetylglycerol from oils and fats. Green Chemistry, 2020, 22, 6345-6350.	4.6	6
29	Spin relaxation induced by interfacial effects in n-GaN/MgO/Co spin injectors. RSC Advances, 2020, 10, 12547-12553.	1.7	7
30	Predicting Crystal Morphology Using a Geometric Descriptor: A Comparative Study of Elemental Crystals with High-Throughput DFT Calculations. Journal of Physical Chemistry C, 2020, 124, 15920-15927.	1.5	6
31	Polymers of Intrinsic Microporosity Having Bulky Substitutes and Cross-Linking for Gas Separation Membranes. ACS Applied Polymer Materials, 2020, 2, 987-995.	2.0	29
32	Zero-energy bound states in the high-temperature superconductors at the two-dimensional limit. Science Advances, 2020, 6, eaax7547.	4.7	25
33	Spectroscopic Imaging of Quasiparticle Bound States Induced by Strong Nonmagnetic Scatterings in One-Unit-Cell FeSe/SrTiO3. Physical Review Letters, 2019, 123, 036801.	2.9	18
34	Inversion Symmetry Breaking Induced Valley Hall Effect in Multilayer WSe₂. ACS Nano, 2019, 13, 9325-9331.	7.3	19
35	Pinpointing the active sites and reaction mechanism of CO oxidation on NiO. Physical Chemistry Chemical Physics, 2019, 21, 17852-17858.	1.3	4
36	Carbon Permeation: The Prerequisite Elementary Step in Iron-Catalyzed Fischerâ€“Tropsch Synthesis. Catalysis Letters, 2019, 149, 645-664.	1.4	19

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37	Mechanism of Graphene Formation via Detonation Synthesis: AÂDFTB Nanoreactor Approach. Journal of Chemical Theory and Computation, 2019, 15, 3654-3665.	2.3	25
38	Enhanced thermal resistance of carbon/phenolic composites by addition of novel nano-g-C3N4. Composites Science and Technology, 2019, 180, 60-70.	3.8	24
39	Resolving a Decade-Long Question of Oxygen Defects in Raman Spectra of Ceria-Based Catalysts at Atomic Level. Journal of Physical Chemistry C, 2019, 123, 18889-18894.	1.5	53
40	Exploration of Properties from Both the Bulk and Surface of Iron Silicides: A Unified Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 11939-11949.	1.5	4
41	Visiting CH4 formation and C1â€¯+â€¯C1 couplings to tune CH4 selectivity on Fe surfaces. Journal of Catalysis, 2019, 372, 217-225.	3.1	19
42	One-pot selective synthesis of azoxy compounds and imines via the photoredox reaction of nitroaromatic compounds and amines in water. Scientific Reports, 2019, 9, 1280.	1.6	10
43	Morphology and Reactivity Evolution of HCP and FCC Ru Nanoparticles under CO Atmosphere. ACS Catalysis, 2019, 9, 2768-2776.	5.5	36
44	Comparison of graphene oxide and graphitic carbon nitride filled carbonâ€“phenolic composites: Thermomechanical properties and role of the strong electronegativity of nanofillers. Journal of Applied Polymer Science, 2018, 135, 46242.	1.3	11
45	Surface Activation of Transition Metal Nanoparticles for Heterogeneous Catalysis: What We Can Learn from Molecular Dynamics. ACS Catalysis, 2018, 8, 3365-3375.	5.5	58
46	First-principles study of charge and magnetic ordering in monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>NbSe</mml:mi><mml:mn>2</mml:mn></mml:msub></m Physical Review B, 2018, 97, .	1.1	38
47	Hydrogen Evolution Reaction on Hybrid Catalysts of Vertical MoS₂ Nanosheets and Hydrogenated Graphene. ACS Catalysis, 2018, 8, 1828-1836.	5.5	180
48	A combined computational and experimental study of the adsorption of sulfur containing molecules on molybdenum disulfide nanoparticles. Journal of Materials Research, 2018, 33, 3589-3603.	1.2	9
49	Tailoring the Electronic Structure and Chemical Activity of Iron via Confining into Two-Dimensional Materials. Journal of Physical Chemistry C, 2018, 122, 24037-24045.	1.5	5
50	Pressure-Induced Phase Engineering of Gold Nanostructures. Journal of the American Chemical Society, 2018, 140, 15783-15790.	6.6	68
51	Extraordinary improvement of ablation resistance of carbon/phenolic composites reinforced with low loading of graphene oxide. Composites Science and Technology, 2018, 167, 53-61.	3.8	40
52	Tuning Gold Nanoparticles with Chelating Ligands for Highly Efficient Electrocatalytic CO₂ Reduction. Angewandte Chemie - International Edition, 2018, 57, 12675-12679.	7.2	108
53	Insight into the Nanoparticle Growth in Supported Ni Catalysts during the Early Stage of CO Hydrogenation Reaction: The Important Role of Adsorbed CO Molecules. ACS Catalysis, 2018, 8, 6367-6374.	5.5	25
54	Product Distribution Control for Glucosamine Condensation: Nuclear Magnetic Resonance (NMR) Investigation Substantiated by Density Functional Calculations. Industrial & Engineering Chemistry Research, 2017, 56, 2925-2934.	1.8	27

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55	Insight into the structure and energy of Mo₂₇S_xO_yclusters. RSC Advances, 2017, 7, 9513-9520.	1.7	20
56	The role of water on the selective decarbonylation of 5-hydroxymethylfurfural over Pd/Al 2 O 3 catalyst: Experimental and DFT studies. Applied Catalysis B: Environmental, 2017, 212, 15-22.	10.8	29
57	In situ ATR-FTIR investigation and theoretical calculation of the interactions of chromate and citrate on the surface of haematite (Î±-Fe₂O₃). RSC Advances, 2017, 7, 41011-41016.	1.7	18
58	Observation of magnetoelastic effects in a quasi-one-dimensional spiral magnet. Physical Review B, 2017, 96, .	1.1	6
59	Mechanism of the self-condensation of GlcNH2: insights from in situ NMR spectroscopy and DFT study. Applied Catalysis B: Environmental, 2017, 202, 420-429.	10.8	22
60	How far away are iron carbide clusters from the bulk?. Physical Chemistry Chemical Physics, 2016, 18, 32944-32951.	1.3	12
61	Density-functional-based tight-binding parameterization of Mo, C, H, O and Si for studying hydrogenation reactions on molybdenum carbide. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	2
62	Application of topological analysis of the electron localization function to the complexes of molybdenum carbide nanoparticles with unsaturated hydrocarbons. Canadian Journal of Chemistry, 2016, 94, 282-292.	0.6	3
63	Molybdenum carbide nanoparticles as catalysts for oil sands upgrading: Dynamics and free-energy profiles. AIP Conference Proceedings, 2015, , .	0.3	0
64	The internal and external factor on coal ash slag viscosity at high temperatures, Part 2: Effect of residual carbon on slag viscosity. Fuel, 2015, 158, 976-982.	3.4	45
65	Molybdenum Carbide Nanocatalysts at Work in the in Situ Environment: A Density Functional Tight-Binding and Quantum Mechanical/Molecular Mechanical Study. Journal of the American Chemical Society, 2015, 137, 4249-4259.	6.6	28
66	Multiscale Modelling of In Situ Oil Sands Upgrading with Molybdenum Carbide Nanoparticles. Challenges and Advances in Computational Chemistry and Physics, 2015, , 415-445.	0.6	2
67	Adsorption of Hexacyclic C₆H₆, C₆H₈, C₆H₁₀, and C₆H₁₂ on a Mo-Terminated Î±-Mo₂C (0001) Surface. Journal of Physical Chemistry C, 2013, 117, 7069-7080.	1.5	26
68	Density functional study of benzene adsorption on the Î±-Mo2C(0001) surface. Structural Chemistry, 2012, 23, 1459-1466.	1.0	16
69	Circular Dichroism Spectroelectrochemical and Voltammetric Studies of Vitamin B2. Electroanalysis, 2001, 13, 1071-1075.	1.5	4