Xiang-Kui Gu

List of Publications by Year
in descending order

46 papers	3,425 citations	218677 26 h-index	189892 50 g-index
52 all docs	52 docs citations	52 times ranked	4918 citing authors

#	Article	IF	Citations
1	Interface-Confined Ferrous Centers for Catalytic Oxidation. Science, 2010, 328, 1141-1144.	12.6	866
2	Water-Mediated Marsâ€"Van Krevelen Mechanism for CO Oxidation on Ceria-Supported Single-Atom Pt₁ Catalyst. ACS Catalysis, 2017, 7, 887-891.	11.2	407
3	Supported Single Pt₁/Au₁ Atoms for Methanol Steam Reforming. ACS Catalysis, 2014, 4, 3886-3890.	11.2	204
4	Disentangling the size-dependent geometric and electronic effects of palladium nanocatalysts beyond selectivity. Science Advances, 2019, 5, eaat6413.	10.3	187
5	Crystalâ€Planeâ€Controlled Selectivity of Cu₂O Catalysts in Propylene Oxidation with Molecular Oxygen. Angewandte Chemie - International Edition, 2014, 53, 4856-4861.	13.8	180
6	Stabilization of Copper Catalysts for Liquidâ€Phase Reactions by Atomic Layer Deposition. Angewandte Chemie - International Edition, 2013, 52, 13808-13812.	13.8	162
7	First-Principles Study on the Origin of the Different Selectivities for Methanol Steam Reforming on Cu(111) and Pd(111). Journal of Physical Chemistry C, 2010, 114, 21539-21547.	3.1	137
8	Engineering the Electronic Structure of Submonolayer Pt on Intermetallic Pd₃Pb via Charge Transfer Boosts the Hydrogen Evolution Reaction. Journal of the American Chemical Society, 2019, 141, 19964-19968.	13.7	99
9	Single Pd Atom Embedded in CeO₂(111) for NO Reduction with CO: A First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 12216-12223.	3.1	98
10	Atomic Layer Deposition Overcoating: Tuning Catalyst Selectivity for Biomass Conversion. Angewandte Chemie - International Edition, 2014, 53, 12132-12136.	13.8	78
11	First-Principles Study of Structure Sensitivity of Ethylene Glycol Conversion on Platinum. ACS Catalysis, 2015, 5, 2623-2631.	11.2	60
12	Theoretical Study of the Role of a Metalâ€"Cation Ensemble at the Oxideâ€"Metal Boundary on CO Oxidation. Journal of Physical Chemistry C, 2012, 116, 7491-7498.	3.1	59
13	Oxygen evolution electrocatalysis using mixed metal oxides under acidic conditions: Challenges and opportunities. Journal of Catalysis, 2020, 388, 130-140.	6.2	59
14	Oxygen Sponges for Electrocatalysis: Oxygen Reduction/Evolution on Nonstoichiometric, Mixed Metal Oxides. Chemistry of Materials, 2018, 30, 2860-2872.	6.7	56
15	Efficient Oxygen Electrocatalysis by Nanostructured Mixed-Metal Oxides. Journal of the American Chemical Society, 2018, 140, 8128-8137.	13.7	49
16	Superior activity of Rh1/ZnO single-atom catalyst for CO oxidation. Chinese Journal of Catalysis, 2019, 40, 1847-1853.	14.0	47
17	Trimethylaluminum and Oxygen Atomic Layer Deposition on Hydroxyl-Free Cu(111). ACS Applied Materials & Interfaces, 2015, 7, 16428-16439.	8.0	39
18	CO Oxidation at the Perimeters of an FeO/Pt(111) Interface and how Water Promotes the Activity: A Firstâ€Principles Study. ChemSusChem, 2012, 5, 871-878.	6.8	37

#	Article	IF	Citations
19	Differentiating Intrinsic Reactivity of Copper, Copperâ€“Zinc Alloy, and Copper/Zinc Oxide Interface for Methanol Steam Reforming by First-Principles Theory. Journal of Physical Chemistry C, 2017, 121, 21553-21559.	3.1	37
20	Following Molecules through Reactive Networks: Surface Catalyzed Decomposition of Methanol on Pd(111), Pt(111), and Ni(111). Journal of Physical Chemistry C, 2014, 118, 12364-12383.	3.1	35
21	Structure evolution of Ptâ€“3d transition metal alloys under reductive and oxidizing conditions and effect on the CO oxidation: a first-principles study. Catalysis Today, 2011, 165, 89-95.	4.4	33
22	Fine cubic Cu2O nanocrystals as highly selective catalyst for propylene epoxidation with molecular oxygen. Nature Communications, 2021, 12, 5921.	12.8	33
23	Design of Ruddlesdenâ€“Popper Oxides with Optimal Surface Oxygen Exchange Properties for Oxygen Reduction and Evolution. ACS Catalysis, 2017, 7, 5912-5920.	11.2	32
24	Engineering Complex, Layered Metal Oxides: High-Performance Nickelate Oxide Nanostructures for Oxygen Exchange and Reduction. ACS Catalysis, 2015, 5, 4013-4019.	11.2	30
25	Design Strategies for Efficient Nonstoichiometric Mixed Metal Oxide Electrocatalysts: Correlating Measurable Oxide Properties to Electrocatalytic Performance. ACS Catalysis, 2019, 9, 10575-10586.	11.2	28
26	First-principles study of single transition metal atoms on ZnO for the water gas shift reaction. Catalysis Science and Technology, 2017, 7, 4294-4301.	4.1	27
27	Fundamental Insights into High-Temperature Water Electrolysis Using Ni-Based Electrocatalysts. Journal of Physical Chemistry C, 2015, 119, 26980-26988.	3.1	26
28	Reaction of Trimethylaluminum with Water on Pt(111) and Pd(111) from 10^{â€“5} to 10^{â€“1} Millibar. Journal of Physical Chemistry C, 2015, 119, 2399-2411.	3.1	21
29	First-Principles and Microkinetic Simulation Studies of the Structure Sensitivity of Cu Catalyst for Methanol Steam Reforming. Journal of Physical Chemistry C, 2018, 122, 10811-10819.	3.1	20
30	Preferential cleavage of C C bonds over C N bonds at interfacial CuO Cu2O sites. Journal of Catalysis, 2015, 330, 458-464.	6.2	18
31	Robust Ruddlesdenâ€Popper phase Sr₃Fe_{1.3}Mo_{0.5}N_{i0.2}O_{7â€Î´} decorated with inâ€situ exsolved Ni nanoparticles as an efficient anode for hydrocarbon fueled solid oxide fuel cells. SusMat, 2022, 2, 487-501.	14.9	18
32	Electrochemical Reduction of CO₂ on Metal-Based Cathode Electrocatalysts of Solid Oxide Electrolysis Cells. Industrial & Engineering Chemistry Research, 2020, 59, 15884-15893.	3.7	17
33	First-Principles Study of High Temperature CO₂ Electrolysis on Transition Metal Electrocatalysts. Industrial & Engineering Chemistry Research, 2017, 56, 6155-6163.	3.7	16
34	One-step synthesis of gasoline fuels from Î³-valerolactone with high selectivity over Cu/HZSM-5 bifunctional catalyst. Applied Catalysis B: Environmental, 2021, 296, 120338.	20.2	16
35	Surface Chemistry of Trimethylaluminum on Pd(111) and Pt(111). Journal of Physical Chemistry C, 2015, 119, 19059-19072.	3.1	14
36	First-principles study of water activation on Cu-ZnO catalysts. Chinese Journal of Catalysis, 2013, 34, 1705-1711.	14.0	11

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37	One-step synthesis of pentane fuel from Î³-valerolactone with high selectivity over a Co/HZSM-5 bifunctional catalyst. Green Chemistry, 2021, 23, 4780-4789.	9.0	10
38	Modulating Catalytic Properties of Targeted Metal Cationic Centers in Nonstochiometric Mixed Metal Oxides for Electrochemical Oxygen Reduction. ACS Energy Letters, 2021, 6, 1065-1072.	17.4	10
39	Ethylene adsorption on Ag(111), Rh(111) and Ir(111) by (meta)-GGA based density functional theory calculations. Chinese Journal of Chemical Physics, 2019, 32, 437-443.	1.3	9
40	Controlling reaction pathways via selective C-O activation for highly efficient biomass oriented-upgrading. Chemical Engineering Journal, 2022, 446, 137404.	12.7	9
41	Characterization and theory of Re films on Pt(111) grown by UHV-CVD. Surface Science, 2015, 640, 2-9.	1.9	8
42	Understanding Surface Catalyzed Decomposition Reactions Using a Chemical Pathway Analysis. Journal of Physical Chemistry C, 2018, 122, 28158-28172.	3.1	8
43	Bimetallic Cu/Rh Catalyst for Preferential Oxidation of CO in H₂: a DFT Study. Journal of Physical Chemistry C, 2021, 125, 19697-19705.	3.1	7
44	Finding Key Factors for Efficient Water and Methanol Activation at Metals, Oxides, MXenes, and Metal/Oxide Interfaces. ACS Catalysis, 2022, 12, 1237-1246.	11.2	5
45	Heterogeneous electrocatalysts for CO2 reduction. Catalysis, 0, , 94-121.	1.0	2
46	RÃ¼cktitelbild: Stabilization of Copper Catalysts for Liquid-Phase Reactions by Atomic Layer Deposition (Angew. Chem. 51/2013). Angewandte Chemie, 2013, 125, 14068-14068.	2.0	1