Chun-Ran Chang

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Single Carbon Vacancy Traps Atomic Platinum for Hydrogen Evolution Catalysis. Journal of the American Chemical Society, 2022, 144, 2171-2178.	13.7	140
2	Design of Single-Atom and Frustrated-Lewis-Pair dual active sites for direct conversion of CH4 and CO2 to acetic acid. Journal of Catalysis, 2022, 408, 206-215.	6.2	18
3	Leaching of palladium atoms from small cluster models during Heck reactions – An experimental and theoretical study. Catalysis Communications, 2022, 165, 106441.	3.3	4
4	Perceptions on the treatment of apparent isotope effects during the analyses of reaction rate and mechanism. Physical Chemistry Chemical Physics, 2022, 24, 15182-15194.	2.8	10
5	Synergy of Pd atoms and oxygen vacancies on In2O3 for methane conversion under visible light. Nature Communications, 2022, 13, .	12.8	105
6	Boosting the thermal stability and catalytic performance by confining Ag single atom sites over antimony-doped tin oxide via atom trapping. Applied Catalysis B: Environmental, 2021, 283, 119625.	20.2	36
7	Highly efficient ammonia synthesis at low temperature over a Ru–Co catalyst with dual atomically dispersed active centers. Chemical Science, 2021, 12, 7125-7137.	7.4	35
8	Gallium nitride catalyzed the direct hydrogenation of carbon dioxide to dimethyl ether as primary product. Nature Communications, 2021, 12, 2305.	12.8	45
9	Screening silica-confined single-atom catalysts for nonoxidative conversion of methane. Journal of Chemical Physics, 2021, 154, 174706.	3.0	6
10	Hierarchically Hollow MnO ₂ @CeO ₂ Heterostructures for NO Oxidation: Remarkably Promoted Activity and SO ₂ Tolerance. ACS Catalysis, 2021, 11, 10988-10996.	11.2	36
11	Silica-Confined Two-Atom Single-Cluster Catalyst for Direct Nonoxidative Conversion of Methane: A DFT Study. Journal of Physical Chemistry C, 2021, 125, 23212-23218.	3.1	3
12	Theoretical Insights into Dual-Metal-Site Catalysts for the Nonoxidative Coupling of Methane. ACS Catalysis, 2021, 11, 13149-13159.	11.2	16
13	Cooperative Catalysis by Multiple Active Centers in Nonoxidative Conversion of Methane. Journal of Physical Chemistry C, 2020, 124, 13656-13663.	3.1	18
14	Role of surface frustrated Lewis pairs on reduced CeO2(110) in direct conversion of syngas. Chinese Journal of Catalysis, 2020, 41, 1906-1915.	14.0	23
15	An oxygen vacancy-rich two-dimensional Au/TiO ₂ hybrid for synergistically enhanced electrochemical N ₂ activation and reduction. Journal of Materials Chemistry A, 2020, 8, 6586-6596.	10.3	54
16	Single-atom Rh/N-doped carbon electrocatalyst for formic acid oxidation. Nature Nanotechnology, 2020, 15, 390-397.	31.5	420
17	Unravelling the Enigma of Nonoxidative Conversion of Methane on Iron Singleâ€Atom Catalysts. Angewandte Chemie, 2020, 132, 18745-18749.	2.0	12
18	Unravelling the Enigma of Nonoxidative Conversion of Methane on Iron Singleâ€Atom Catalysts. Angewandte Chemie - International Edition, 2020, 59, 18586-18590.	13.8	44

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19	Facet-dependent catalytic activities of Pd/rGO: Exploring dehydrogenation mechanism of dodecahydro-N-ethylcarbazole. Applied Catalysis B: Environmental, 2020, 266, 118658.	20.2	56
20	Gas-Phase Mechanism Study of Methane Nonoxidative Conversion by ReaxFF Method. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2020, .	4.9	3
21	Synergy of the catalytic activation on Ni and the CeO ₂ –TiO ₂ /Ce ₂ Ti ₂ O ₇ stoichiometric redox cycle for dramatically enhanced solar fuel production. Energy and Environmental Science, 2019. 12. 767-779.	30.8	90
22	Dynamic Frustrated Lewis Pairs on Ceria for Direct Nonoxidative Coupling of Methane. ACS Catalysis, 2019, 9, 5523-5536.	11.2	54
23	Ethylene-glycol ligand environment facilitates highly efficient hydrogen evolution of Pt/CoP through proton concentration and hydrogen spillover. Energy and Environmental Science, 2019, 12, 2298-2304.	30.8	227
24	Hydrogen activation enabled by the interfacial frustrated Lewis pairs on cobalt borate nanosheets. Journal of Catalysis, 2019, 372, 142-150.	6.2	27
25	Engineering the electronic structure of single atom Ru sites via compressive strain boosts acidic water oxidation electrocatalysis. Nature Catalysis, 2019, 2, 304-313.	34.4	757
26	A DFT study on the enthalpies of thermite reactions and enthalpies of formation of metal composite oxide. Chemical Physics, 2018, 507, 19-27.	1.9	15
27	Theoretical studies on copper-catalyzed arylation of nitrogen heterocycles from benzenediazonium acetate under ligand-free conditions. Journal of Organometallic Chemistry, 2018, 864, 50-57.	1.8	10
28	Understanding All-Solid Frustrated-Lewis-Pair Sites on CeO ₂ from Theoretical Perspectives. ACS Catalysis, 2018, 8, 546-554.	11.2	135
29	In situ encapsulation of iron(0) for solar thermochemical syngas production over iron-based perovskite material. Communications Chemistry, 2018, 1, .	4.5	55
30	Semi-solid and solid frustrated Lewis pair catalysts. Chemical Society Reviews, 2018, 47, 5541-5553.	38.1	102
31	Mechanistic investigations of Co(II)-Catalyzed C-N coupling reactions. Journal of Organometallic Chemistry, 2018, 868, 144-153.	1.8	16
32	Single-Walled Carbon Nanotube Induced Optimized Electron Polarization of Rhodium Nanocrystals To Develop an Interface Catalyst for Highly Efficient Electrocatalysis. ACS Catalysis, 2018, 8, 8092-8099.	11.2	82
33	Solid frustrated-Lewis-pair catalysts constructed by regulations on surface defects of porous nanorods of CeO2. Nature Communications, 2017, 8, 15266.	12.8	272
34	Modulating electronic structure of CoP electrocatalysts towards enhanced hydrogen evolution by Ce chemical doping in both acidic and basic media. Nano Energy, 2017, 38, 290-296.	16.0	212
35	Stepâ€Edge Assisted Direct Linear Alkane Coupling. Chemistry - A European Journal, 2017, 23, 6185-6189.	3.3	26
36	Trends in water-promoted oxygen dissociation on the transition metal surfaces from first principles. Physical Chemistry Chemical Physics, 2017, 19, 2364-2371.	2.8	39

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37	Design of N-Coordinated Dual-Metal Sites: A Stable and Active Pt-Free Catalyst for Acidic Oxygen Reduction Reaction. Journal of the American Chemical Society, 2017, 139, 17281-17284.	13.7	1,220
38	The promotional role of water in heterogeneous catalysis: mechanism insights from computational modeling. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 679-693.	14.6	58
39	Mechanistic Insights on Ternary Ni _{2â^²} <i>_x</i> Co <i>_x</i> P for Hydrogen Evolution and Their Hybrids with Graphene as Highly Efficient and Robust Catalysts for Overall Water Splitting. Advanced Functional Materials, 2016, 26, 6785-6796.	14.9	500
40	Inside Cover Image, Volume 6, Issue 6. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, ii.	14.6	0
41	Mechanistic Insights into Propene Epoxidation with O ₂ –H ₂ O Mixture on Au ₇ /α-Al ₂ O ₃ : A Hydroproxyl Pathway from ab Initio Molecular Dynamics Simulations. ACS Catalysis, 2016, 6, 2525-2535.	11.2	70
42	High Catalytic Activity and Chemoselectivity of Sub-nanometric Pd Clusters on Porous Nanorods of CeO ₂ for Hydrogenation of Nitroarenes. Journal of the American Chemical Society, 2016, 138, 2629-2637.	13.7	387
43	Theoretical Studies on the Synergetic Effects of Au–Pd Bimetallic Catalysts in the Selective Oxidation of Methanol. Journal of Physical Chemistry C, 2015, 119, 16072-16081.	3.1	45
44	A theoretical study on the catalytic role of water in methanol steam reforming on PdZn(111). Catalysis Science and Technology, 2015, 5, 2935-2944.	4.1	37
45	Visible-Light-Activated Suzuki–Miyaura Coupling Reactions of Aryl Chlorides over the Multifunctional Pd/Au/Porous Nanorods of CeO ₂ Catalysts. ACS Catalysis, 2015, 5, 6481-6488.	11.2	126
46	Hydrogenation of molecular oxygen to hydroperoxyl: An alternative pathway for O2 activation on nanogold catalysts. Nano Research, 2015, 8, 3737-3748.	10.4	34
47	Ultrathin rhodium nanosheets. Nature Communications, 2014, 5, 3093.	12.8	428
48	A Water-Promoted Mechanism of Alcohol Oxidation on a Au(111) Surface: Understanding the Catalytic Behavior of Bulk Gold. ACS Catalysis, 2013, 3, 1693-1699.	11.2	118
49	Nitric acid catalyzed hydrolysis of SO3 in the formation of sulfuric acid: A theoretical study. Chemical Physics Letters, 2013, 581, 26-29.	2.6	37
50	Theoretical Studies on Gas-Phase Reactions of Sulfuric Acid Catalyzed Hydrolysis of Formaldehyde and Formaldehyde with Sulfuric Acid and H ₂ SO ₄ ···H ₂ O Complex. Journal of Physical Chemistry A, 2013, 117, 5106-5116.	2.5	69
51	Theoretical study on the leaching of palladium in a CO atmosphere. Catalysis Science and Technology, 2012, 2, 2238.	4.1	18
52	Theoretical investigations of the catalytic role of water in propene epoxidation on gold nanoclusters: A hydroperoxyl-mediated pathway. Nano Research, 2011, 4, 131-142.	10.4	98
53	Structural Characterization and Thermal Behavior of 1â€Aminoâ€1â€methylaminoâ€2,2â€dinitroethylene. Chines Journal of Chemistry, 2010, 28, 583-588.	e 4.9	15
54	Nonâ€isothermal Decomposition Kinetics, Specific Heat Capacity and Adiabatic Timeâ€toâ€explosion of 1â€Aminoâ€1â€hydrazinoâ€2,2â€dinitroethylene (AHDNE). Chinese Journal of Chemistry, 2009, 27, 665-671.	4.9	18

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55	Preparation, Crystal Structure and Theoretical Calculation of G(FOX-7). Chinese Journal of Chemistry, 2008, 26, 495-499.	4.9	30
56	Molecular Structure, Theoretical Calculation and Thermal Behavior of DAG(NTO). Chinese Journal of Chemistry, 2008, 26, 1549-1554.	4.9	5
57	Thermal behavior, specific heat capacity and adiabatic time-to-explosion of G(FOX-7). Journal of Hazardous Materials, 2008, 158, 333-339.	12.4	76
58	Molecular structure, theoretical calculation and thermal behavior of 2-(1,1-dinitromethylene)-1,3-diazepentane. Journal of Molecular Structure, 2008, 891, 340-345.	3.6	32