Li-Hui Ou

List of Publications by Year
in descending order

33 papers	496 citations	687220 13 h-index	677027 22 g-index
34 all docs	34 docs citations	34 times ranked	810 citing authors

#	Article	IF	Citations
1	Theoretical insights into the origin of promoter effect of alkali metals on Au-catalyzed nitrogen electroreduction. Chemical Physics Letters, 2022, 789, 139320.	1.2	3
2	Theoretical insights into effect of surface composition of Pt-Ru bimetallic catalysts on CH3OH oxidation: mechanistic considerations. Journal of Molecular Modeling, 2022, 28, 149.	0.8	0
3	Solid-Phase Synthesis of Non-metal (S, N)-Doped Tin Oxide Nanopowders at Room Temperature and its Photodegradation Properties for Wastewater of Biomass Treatment. Journal of Inorganic and Organometallic Polymers and Materials, 2022, 32, 2748-2762.	1.9	3
4	Mechanism for CO2 electroreduction into C2 products at the low overpotential: Theoretical insights from an improved electrode/solution interface model. Surface Science, 2021, 705, 121782.	0.8	9
5	Theoretical insights into the promotion effect of alkali metal cations on the electroreduction mechanism of CO₂ into C₁ products at the Cu(111)/H₂O interface. New Journal of Chemistry, 2021, 45, 15582-15593.	1.4	2
6	Theoretical Insights into Potential-Dependent Câ€“C Bond Formation Mechanisms during CO₂ Electroreduction into C₂ Products on Cu(100) at Simulated Electrochemical Interfaces. ACS Omega, 2021, 6, 17839-17847.	1.6	17
7	Theoretical insights into the electroreduction mechanism of N₂ to NH₃ from an improved Au(111)/H₂O interface model. RSC Advances, 2021, 11, 17828-17839.	1.7	6
8	Theoretical insights into the effect of the overpotential on CO electroreduction mechanisms on Cu(111): regulation and application of electrode potentials from a CO coverage-dependent electrochemical model. Physical Chemistry Chemical Physics, 2020, 22, 62-73.	1.3	3
9	Density Functional Studies on Photophysical Properties of Boron-Pyridyl-Imino-Isoindoline Dyes: Effect of the Fusion. ACS Omega, 2020, 5, 21067-21075.	1.6	3
10	Mechanistic insights into potential dependence of CO electrochemical reduction into C1 products based on a H coverage-dependent Cu(111)/H2O interface model. Physical Chemistry Chemical Physics, 2020, 22, 20444-20452.	1.3	5
11	Potential-Dependent Competitive Electroreduction of CO₂ into CO and Formate on Cu(111) from an Improved H Coverage-Dependent Electrochemical Model with Explicit Solvent Effect. ACS Omega, 2020, 5, 12735-12744.	1.6	8
12	Potential-Dependent CO2 Electroreduction Pathways on Cu(111) Based on an Improved Electrode/Aqueous Interface Model: Determination of the Origin of the Overpotentials. ACS Omega, 2019, 4, 17269-17278.	1.6	4
13	Mechanistic Understanding of the Effect of Surface Composition of Ptâ€Ru Bimetallic Alloy Electrocatalysts on HCOOH Oxidation Pathways at Acid Electrochemical Interface. ChemistrySelect, 2019, 4, 7190-7199.	0.7	0
14	Mechanistic study on Cu-catalyzed CO₂ electroreduction into CH₄ at simulated low overpotentials based on an improved electrochemical model. Physical Chemistry Chemical Physics, 2019, 21, 15531-15540.	1.3	17
15	New Insights into the Pt-Catalyzed CH₃OH Oxidation Mechanism: First-Principle Considerations on Thermodynamics, Kinetics, and Reversible Potentials. ACS Omega, 2018, 3, 886-897.	1.6	12
16	Mechanistic Study of Pt-Catalyzed Electrooxidation of HCOOH in Acid Medium: Kinetic Considerations on the Effect of Solvation. Journal of Physical Chemistry C, 2018, 122, 24871-24884.	1.5	16
17	The origin of CO2 electroreduction into C1 and C2 species: Mechanistic understanding on the product selectivity of Cu single-crystal faces. Chemical Physics Letters, 2018, 710, 175-179.	1.2	16
18	Theoretical Insights into the Effect of Solvation and Sublayer Ru on Pt-Catalytic CH3OH Oxidation Mechanisms in the Aqueous Phase. Journal of Physical Chemistry C, 2018, 122, 14554-14565.	1.5	15

#	Article	IF	Citations
19	Theoretical insight into effect of doping of transition metalÂM (M = Ni, Pd and Pt) on CO₂ reduction pathways on Cu(111) and understanding of origin of electrocatalytic activity. RSC Advances, 2017, 7, 11938-11950.	1.7	20
20	DFT-based study on the optimal CH3OH decomposition pathways in aqueous-phase: Homolysis versus heterolysis. Chemical Physics Letters, 2017, 679, 66-70.	1.2	6
21	Mechanistic insight into effect of doping of Ni on CO2 reduction on the (111) facet of Cu: thermodynamic and kinetic analyses of the elementary steps. Journal of Molecular Modeling, 2016, 22, 246.	0.8	5
22	Theoretical insights into the alkaline metal M (MÂ= Na and Cs) promotion mechanism for CO₂ activation on the Cu(111) surface. RSC Advances, 2016, 6, 67866-67874.	1.7	8
23	New reduction mechanism of CO dimer by hydrogenation to C₂H₄ on a Cu(100) surface: theoretical insight into the kinetics of the elementary steps. RSC Advances, 2015, 5, 96281-96289.	1.7	19
24	Design of Pd-Based Bimetallic Catalysts for ORR: A DFT Calculation Study. Journal of Chemistry, 2015, 2015, 1-11.	0.9	28
25	New insights into the effects of alloying Pt with Ni on oxygen reduction reaction mechanisms in acid medium: a first-principles study. Journal of Molecular Modeling, 2015, 21, 281.	0.8	4
26	Chemical and electrochemical hydrogenation of CO₂ to hydrocarbons on Cu single crystal surfaces: insights into the mechanism and selectivity from DFT calculations. RSC Advances, 2015, 5, 57361-57371.	1.7	32
27	DFT calculation analysis of oxygen reduction activity and stability of bimetallic catalysts with Pt-segregated surface. Science China Chemistry, 2015, 58, 586-592.	4.2	12
28	The origin of enhanced electrocatalytic activity of Ptâ€“M (M=Fe, Co, Ni, Cu, and W) alloys in PEM fuel cell cathodes: A DFT computational study. Computational and Theoretical Chemistry, 2014, 1048, 69-76.	1.1	43
29	Comparative Study of Oxygen Reduction Reaction Mechanisms on the Pd(111) and Pt(111) Surfaces in Acid Medium by DFT. Journal of Physical Chemistry C, 2013, 117, 1342-1349.	1.5	59
30	Efficient and Superiorly Durable Pt-Lean Electrocatalysts of Ptâ^'W Alloys for the Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2011, 115, 2162-2168.	1.5	51
31	Density functional theory (DFT)-based modified embedded atom method potentials: Bridging the gap between nanoscale theoretical simulations and DFT calculations. Science China Chemistry, 2010, 53, 411-418.	4.2	3
32	First-Principle Study of the Adsorption and Dissociation of O₂ on Pt(111) in Acidic Media. Journal of Physical Chemistry C, 2009, 113, 20657-20665.	1.5	66
33	Theoretical Evaluation of Effect of Bimetallic Au-based Alloy Catalysts on Initial N2 Electroreduction Pathways. Physical Chemistry Chemical Physics, 0, , .	1.3	1