Wei-Xue Li

List of Publications by Year in Descending Order

121 papers	7,790 citations	43 h-index	87 g-index
130 ext. papers	9,293 ext. citations	8 avg, IF	6.11 L-index

#	Paper	IF	Citations
121	Finding Key Factors for Efficient Water and Methanol Activation at Metals, Oxides, MXenes, and Metal/Oxide Interfaces.. *ACS Catalysis*, **2022**, 12, 1237-1246	13.1	0
120	Atomically dispersed Ir/□MoC catalyst with high metal loading and thermal stability for water-promoted hydrogenation reaction.. *National Science Review*, **2022**, 9, nwab026	10.8	18
119	First-Principles Study of Oxygen-Induced Disintegration and Ripening of Late Transition Metal Nanoparticles on Rutile-TiO2(110). *Journal of Physical Chemistry C*, **2022**, 126, 8056-8064	3.8	
118	Sabatier principle of metal-support interaction for design of ultrastable metal nanocatalysts. *Science*, **2021**, 374, 1360-1365	33.3	30
117	Boosting Activity and Stability of Metal Single-Atom Catalysts via Regulation of Coordination Number and Local Composition. *Journal of the American Chemical Society*, **2021**, 143, 18854-18858	16.4	23
116	K-Edge XANES Investigation of Fe-Based Oxides by Density Functional Theory Calculations. *Journal of Physical Chemistry C*, **2021**, 125, 26229-26239	3.8	1
115	Bimetallic monolayer catalyst breaks the activity□selectivity trade-off on metal particle size for efficient chemoselective hydrogenations. *Nature Catalysis*, **2021**, 4, 840-849	36.5	19
114	Intrinsic Electrocatalytic Activity for Oxygen Evolution of Crystalline 3d-Transition Metal Layered Double Hydroxides. *Angewandte Chemie*, **2021**, 133, 14567-14578	3.6	8
113	Intrinsic Electrocatalytic Activity for Oxygen Evolution of Crystalline 3d-Transition Metal Layered Double Hydroxides. *Angewandte Chemie - International Edition*, **2021**, 60, 14446-14457	16.4	40
112	Crystallographic and morphological sensitivity of N2 activation over ruthenium. *Chinese Journal of Chemical Physics*, **2021**, 34, 263-272	0.9	0
111	Synergizing metal-support interactions and spatial confinement boosts dynamics of atomic nickel for hydrogenations. *Nature Nanotechnology*, **2021**, 16, 1141-1149	28.7	40
110	Hydroxyl improving the activity, selectivity and stability of supported Ni single atoms for selective semi-hydrogenation. *Chemical Science*, **2021**, 12, 10290-10298	9.4	4
109	Water enables mild oxidation of methane to methanol on gold single-atom catalysts. *Nature Communications*, **2021**, 12, 1218	17.4	44
108	Quantification of critical particle distance for mitigating catalyst sintering. *Nature Communications*, **2021**, 12, 4865	17.4	13
107	Bimetallic Cu/Rh Catalyst for Preferential Oxidation of CO in H2: a DFT Study. *Journal of Physical Chemistry C*, **2021**, 125, 19697-19705	3.8	2
106	Bridge sulfur vacancies in MoS2 catalyst for reverse water gas shift: A first-principles study. *Applied Surface Science*, **2021**, 561, 149925	6.7	5
105	In-situ structure and catalytic mechanism of NiFe and CoFe layered double hydroxides during oxygen evolution. *Nature Communications*, **2020**, 11, 2522	17.4	273

104	Surface Iron Species in Palladium-Iron Intermetallic Nanocrystals that Promote and Stabilize CO Methanation. *Angewandte Chemie - International Edition*, **2020**, 59, 14434-14442	16.4	22
103	Probing surface defects of ZnO using formaldehyde. *Journal of Chemical Physics*, **2020**, 152, 074714	3.9	4
102	Compensation between Surface Energy and hcp/fcc Phase Energy of Late Transition Metals from First-Principles Calculations. *Journal of Physical Chemistry C*, **2020**, 124, 11005-11014	3.8	13
101	Surface Iron Species in Palladium□Iron Intermetallic Nanocrystals that Promote and Stabilize CO2 Methanation. *Angewandte Chemie*, **2020**, 132, 14542-14550	3.6	6
100	Machine-learning adsorption on binary alloy surfaces for catalyst screening. *Chinese Journal of Chemical Physics*, **2020**, 33, 703-711	0.9	0
99	Ligand Stabilized Ni Catalyst for Efficient CO Oxidation. *ChemPhysChem*, **2020**, 21, 2417-2425	3.2	2
98	Morphology Evolution of FCC and HCP Cobalt Induced by a CO Atmosphere from Ab Initio Thermodynamics. *Journal of Physical Chemistry C*, **2020**, 124, 23200-23209	3.8	3
97	CO activation and methanation mechanism on hexagonal close-packed Co catalysts: effect of functionals, carbon deposition and surface structure. *Catalysis Science and Technology*, **2020**, 10, 3387-3398	5.5	0
96	Single Ru Sites-Embedded Rutile TiO2 Catalyst for Non-Oxidative Direct Conversion of Methane: A First-Principles Study. *Journal of Physical Chemistry C*, **2019**, 123, 14391-14397	3.8	9
95	Adsorption Features of Formaldehyde on TiO(110) Surface Probed by High-Resolution Scanning Tunnelling Microscopy. *Journal of Physical Chemistry Letters*, **2019**, 10, 3352-3358	6.4	8
94	Metal-support interaction controlled migration and coalescence of supported particles. *Science China Technological Sciences*, **2019**, 62, 762-772	3.5	6
93	Engineering the electronic structure of single atom Ru sites via compressive strain boosts acidic water oxidation electrocatalysis. *Nature Catalysis*, **2019**, 2, 304-313	36.5	420
92	Influence of Cobalt Crystal Structures on Activation of Nitrogen Molecule: A First-Principles Study. *Journal of Physical Chemistry C*, **2019**, 123, 10956-10966	3.8	7
91	Influence of Crystal Facet and Phase of Titanium Dioxide on Ostwald Ripening of Supported Pt Nanoparticles from First-Principles Kinetics. *Journal of Physical Chemistry C*, **2019**, 123, 11020-11031	3.8	17
90	Interplay Between Site Activity and Density of BCC Iron for Ammonia Synthesis Based on First-Principles Theory. *ChemCatChem*, **2019**, 11, 1928-1934	5.2	6
89	Carbon Monoxide Activation on Cobalt Carbide for Fischer□Tropsch Synthesis from First-Principles Theory. *ACS Catalysis*, **2019**, 9, 8093-8103	13.1	25
88	Nitrogen-doped graphene layers for electrochemical oxygen reduction reaction boosted by lattice strain. *Journal of Catalysis*, **2019**, 378, 113-120	7.3	10
87	First-principles investigation of electrochemical dissolution of Pt nanoparticles and kinetic simulation. *Journal of Chemical Physics*, **2019**, 151, 234711	3.9	6

86	Engineering the Electronic Structure of Submonolayer Pt on Intermetallic PdPb via Charge Transfer Boosts the Hydrogen Evolution Reaction. *Journal of the American Chemical Society*, **2019**, 141, 19964-19968	16.4	71
85	First-Principles Kinetic Study for Ostwald Ripening of Late Transition Metals on TiO2(110). *Journal of Physical Chemistry C*, **2019**, 123, 1160-1169	3.8	13
84	Surface and interface design for heterogeneous catalysis. *Physical Chemistry Chemical Physics*, **2019**, 21, 523-536	3.6	29
83	Disentangling the size-dependent geometric and electronic effects of palladium nanocatalysts beyond selectivity. *Science Advances*, **2019**, 5, eaat6413	14.3	102
82	First-principles kinetics study of carbon monoxide promoted Ostwald ripening of Au particles on FeO/Pt(111). *Journal of Energy Chemistry*, **2019**, 30, 108-113	12	8
81	Influence of Particle Size Distribution on Lifetime and Thermal Stability of Ostwald Ripening of Supported Particles. *ChemCatChem*, **2018**, 10, 2900-2907	5.2	18
80	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	3.8	12
79	Theoretical Investigation of Metal-Support Interactions on Ripening Kinetics of Supported Particles. *ChemNanoMat*, **2018**, 4, 510-517	3.5	10
78	First-Principles microkinetic study of methanol synthesis on Cu(221) and ZnCu(221) surfaces. *Chinese Journal of Chemical Physics*, **2018**, 31, 284-290	0.9	6
77	Understanding Surface Catalyzed Decomposition Reactions Using a Chemical Pathway Analysis. *Journal of Physical Chemistry C*, **2018**, 122, 28158-28172	3.8	5
76	Structures and stability of adsorbed methanol on TiO2(110) surface studied by ab initio thermodynamics and kinetic Monte Carlo simulation. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	2
75	Metal-Free Nitrogen- and Boron-Codoped Mesoporous Carbons for Primary Amides Synthesis from Primary Alcohols via Direct Oxidative Dehydrogenation. *ACS Catalysis*, **2018**, 8, 9936-9944	13.1	33
74	Chemical Insights into the Design and Development of Face-Centered Cubic Ruthenium Catalysts for Fischer-Tropsch Synthesis. *Journal of the American Chemical Society*, **2017**, 139, 2267-2276	16.4	104
73	Reconstruction of the Wet Chemical Synthesis Process: The Case of Fe5C2 Nanoparticles. *Journal of Physical Chemistry C*, **2017**, 121, 5154-5160	3.8	19
72	Phase-Selective Syntheses of Cobalt Telluride Nanofleeces for Efficient Oxygen Evolution Catalysts. *Angewandte Chemie - International Edition*, **2017**, 56, 7769-7773	16.4	108
71	First-principles study of structure sensitivity of chain growth and selectivity in Fischer‐Tropsch synthesis using HCP cobalt catalysts. *Catalysis Science and Technology*, **2017**, 7, 2967-2977	5.5	22
70	First-principles study of single transition metal atoms on ZnO for the water gas shift reaction. *Catalysis Science and Technology*, **2017**, 7, 4294-4301	5.5	20
69	Carbon induced selective regulation of cobalt-based Fischer-Tropsch catalysts by ethylene treatment. *Faraday Discussions*, **2017**, 197, 207-224	3.6	12

68	Water-Mediated Mars–Van Krevelen Mechanism for CO Oxidation on Ceria-Supported Single-Atom Pt1 Catalyst. *ACS Catalysis*, **2017**, 7, 887-891	13.1	255
67	Differentiating Intrinsic Reactivity of Copper, Copper–Zinc Alloy, and Copper/Zinc Oxide Interface for Methanol Steam Reforming by First-Principles Theory. *Journal of Physical Chemistry C*, **2017**, 121, 21553-21559	3.8	17
66	The most active Cu facet for low-temperature water gas shift reaction. *Nature Communications*, **2017**, 8, 488	17.4	98
65	Influence of nickel(II) oxide surface magnetism on molecule adsorption: A first-principles study. *Chinese Journal of Catalysis*, **2017**, 38, 1736-1748	11.3	2
64	CO Dissociation on Face-Centered Cubic and Hexagonal Close-Packed Nickel Catalysts: A First-Principles Study. *Journal of Physical Chemistry C*, **2016**, 120, 24895-24903	3.8	35
63	Theoretical study of crystal phase effect in heterogeneous catalysis. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 571-583	7.9	27
62	Establishing and Understanding Adsorption-Energy Scaling Relations with Negative Slopes. *Journal of Physical Chemistry Letters*, **2016**, 7, 5302-5306	6.4	30
61	Direct Imaging Single Methanol Molecule Photocatalysis on Titania. *Journal of Physical Chemistry C*, **2015**, 119, 17748-17754	3.8	34
60	Robust Phase Control through Hetero-Seeded Epitaxial Growth for Face-Centered Cubic Pt@Ru Nanotetrahedrons with Superior Hydrogen Electro-Oxidation Activity. *Journal of Physical Chemistry C*, **2015**, 119, 17697-17706	3.8	60
59	High Alcohols Synthesis via Fischer–Tropsch Reaction at Cobalt Metal/Carbide Interface. *ACS Catalysis*, **2015**, 5, 3620-3624	13.1	172
58	A First-Principles Study of Carbon–Oxygen Bond Scission in Multiatomic Molecules on Flat and Stepped Metal Surfaces. *ChemCatChem*, **2014**, 6, 1755-1762	5.2	11
57	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	3.8	28
56	Stability of polar ZnO surfaces studied by pair potential method and local energy density method. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	7
55	Supported Single Pt1/Au1 Atoms for Methanol Steam Reforming. *ACS Catalysis*, **2014**, 4, 3886-3890	13.1	158
54	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	3.8	88
53	CO- and NO-Induced Disintegration and Redispersion of Three-Way Catalysts Rhodium, Palladium, and Platinum: An ab Initio Thermodynamics Study. *Journal of Physical Chemistry C*, **2014**, 118, 9588-9597	3.8	43
52	Crystal-plane-controlled selectivity of Cu(2)O catalysts in propylene oxidation with molecular oxygen. *Angewandte Chemie - International Edition*, **2014**, 53, 4856-61	16.4	152
51	Structure sensitivity of CO methanation on Co (0001), and surfaces: Density functional theory calculations. *Catalysis Today*, **2013**, 215, 36-42	5.3	60

50	Crystallographic dependence of CO activation on cobalt catalysts: HCP versus FCC. *Journal of the American Chemical Society*, **2013**, 135, 16284-7	16.4	269
49	Adsorbed CO induced change of the adsorption site and charge of Au adatoms on FeO(111)/Ru(0001). *Chinese Journal of Catalysis*, **2013**, 34, 1820-1825	11.3	2
48	First-principles study of water activation on Cu-ZnO catalysts. *Chinese Journal of Catalysis*, **2013**, 34, 1705-1711	11.3	9
47	Platinum-modulated cobalt nanocatalysts for low-temperature aqueous-phase Fischer-Tropsch synthesis. *Journal of the American Chemical Society*, **2013**, 135, 4149-58	16.4	98
46	Atomistic theory of Ostwald ripening and disintegration of supported metal particles under reaction conditions. *Journal of the American Chemical Society*, **2013**, 135, 1760-71	16.4	284
45	Growth of Single- and Bilayer ZnO on Au(111) and Interaction with Copper. *Journal of Physical Chemistry C*, **2013**, 117, 11211-11218	3.8	89
44	Mechanistic studies of water electrolysis and hydrogen electro-oxidation on high temperature ceria-based solid oxide electrochemical cells. *Journal of the American Chemical Society*, **2013**, 135, 11572-9	16.4	75
43	Force reversed method for locating transition states. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	50
42	Theoretical Study of the Role of a Metal Cation Ensemble at the Oxide Metal Boundary on CO Oxidation. *Journal of Physical Chemistry C*, **2012**, 116, 7491-7498	3.8	54
41	Structural and electronic properties of cobalt carbide Co2C and its surface stability: Density functional theory study. *Surface Science*, **2012**, 606, 598-604	1.8	65
40	In- and Out-Dependent Interactions of Iron with Carbon Nanotubes. *Journal of Physical Chemistry C*, **2012**, 116, 16461-16466	3.8	26
39	CO oxidation at the perimeters of an FeO/Pt(111) interface and how water promotes the activity: a first-principles study. *ChemSusChem*, **2012**, 5, 871-8	8.3	30
38	Size-selective carbon nanoclusters as precursors to the growth of epitaxial graphene. *Nano Letters*, **2011**, 11, 424-30	11.5	128
37	Toward N-Doped Graphene via Solvothermal Synthesis. *Chemistry of Materials*, **2011**, 23, 1188-1193	9.6	872
36	Carbon chain growth by formyl insertion on rhodium and cobalt catalysts in syngas conversion. *Angewandte Chemie - International Edition*, **2011**, 50, 5335-8	16.4	93
35	Carbon monoxide adsorption and dissociation on Mn-decorated Rh(111) and Rh(553) surfaces: A first-principles study. *Catalysis Today*, **2011**, 160, 228-233	5.3	26
34	Structure evolution of Pt3d transition metal alloys under reductive and oxidizing conditions and effect on the CO oxidation: a first-principles study. *Catalysis Today*, **2011**, 165, 89-95	5.3	30
33	In situ oxidation study of Pt(110) and its interaction with CO. *Journal of the American Chemical Society*, **2011**, 133, 20319-25	16.4	115

32	Rh-Decorated Cu Alloy Catalyst for Improved C2 Oxygenate Formation from Syngas. *Journal of Physical Chemistry C*, **2011**, 115, 18247-18256	3.8	59
31	First-principles study of the adsorption of Au atoms and Au2 and Au4 clusters on FeO/Pt(111). *Physical Review B*, **2011**, 84,	3.3	19
30	Theory of nitride oxide adsorption on transition metal (111) surfaces: a first-principles investigation. *Physical Chemistry Chemical Physics*, **2010**, 12, 2459-70	3.6	49
29	Density functional theory and ab initio molecular dynamics study of NO adsorption on Pd(111) and Pt(111) surfaces. *Physical Review B*, **2010**, 81,	3.3	15
28	Band structure and Fermi surface of atomically uniform lead films. *New Journal of Physics*, **2010**, 12, 113034	3.7	1
27	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	3.8	120
26	First-principles study of hydrogen absorption on Mg(0001) and formation of magnesium hydride. *Physical Review B*, **2010**, 81,	3.3	25
25	Interface-confined ferrous centers for catalytic oxidation. *Science*, **2010**, 328, 1141-4	33.3	743
24	Density functional theory study of the energetics, electronic structure, and core-level shifts of NO adsorption on the Pt(111) surface. *Physical Review B*, **2009**, 79,	3.3	43
23	Reversible structural modulation of Fe-Pt bimetallic surfaces and its effect on reactivity. *ChemPhysChem*, **2009**, 10, 1013-6	3.2	63
22	A first-principles study on the behavior of HCl inside SWCNT. *Computational and Theoretical Chemistry*, **2009**, 905, 44-47		11
21	Cooperative activation in ring-opening hydrolysis of epoxides by Co-salen complexes: A first principle study. *Chemical Physics Letters*, **2009**, 470, 259-263	2.5	19
20	First-Principles Investigation of Surface and Subsurface H Adsorption on Ir(111). *Journal of Physical Chemistry C*, **2009**, 113, 21361-21367	3.8	28
19	First-Principles Study of Carbon Monoxide Oxidation on Ag(111) in Presence of Subsurface Oxygen and Stepped Ag(221). *Journal of Physical Chemistry C*, **2009**, 113, 8266-8272	3.8	27
18	The Effect of Water on the CO Oxidation on Ag(111) and Au(111) Surfaces: A First-Principle Study. *Journal of Physical Chemistry C*, **2008**, 112, 17303-17310	3.8	143
17	Atomic and molecular adsorption on RhMn alloy surface: a first principles study. *Journal of Chemical Physics*, **2008**, 129, 244711	3.9	12
16	Hydrolysis of ball milling AlB_2H_7 hydride and AlB_3 salt mixture for hydrogen generation. *Journal of Alloys and Compounds*, **2008**, 460, 125-129	5.7	77
15	Framework Fe Ions in Fe-ZSM-5 Zeolite Studied by UV Resonance Raman Spectroscopy and Density Functional Theory Calculations. *Journal of Physical Chemistry C*, **2008**, 112, 16036-16041	3.8	51

14	Oxidation of platinum surfaces and reaction with carbon monoxide. *Journal of Physics Condensed Matter*, **2008**, 20, 184022	1.8	12
13	Wavevector-dependent quantum-size effect in electron decay length at Pb thin film surfaces. *Applied Physics Letters*, **2008**, 93, 093105	3.4	18
12	Modulating the reactivity of Ni-containing Pt(111)-skin catalysts by density functional theory calculations. *Journal of Chemical Physics*, **2008**, 128, 194707	3.9	43
11	Step enhanced dehydrogenation of ethanol on Rh. *Surface Science*, **2008**, 602, 3057-3063	1.8	20
10	Unique reactivity of confined metal atoms on a silicon substrate. *ChemPhysChem*, **2008**, 9, 975-9	3.2	23
9	First Principle Study of Ethanol Adsorption and Formation of Hydrogen Bond on Rh(111) Surface. *Journal of Physical Chemistry C*, **2007**, 111, 7403-7410	3.8	44
8	The improved electrochemical properties of novel La-Mg-Ni-based hydrogen storage composites. *Electrochimica Acta*, **2007**, 52, 6700-6706	6.7	30
7	Experimental observation of quantum oscillation of surface chemical reactivities. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 9204-8	11.5	113
6	Density functional theory study of CHx (x=1-3) adsorption on clean and CO precovered Rh(111) surfaces. *Journal of Chemical Physics*, **2007**, 127, 024705	3.9	15
5	Insights into the function of silver as an oxidation catalyst by ab initio atomistic thermodynamics. *Physical Review B*, **2003**, 68,	3.3	157
4	Why is a noble metal catalytically active? The role of the O-Ag interaction in the function of silver as an oxidation catalyst. *Physical Review Letters*, **2003**, 90, 256102	7.4	158
3	Subsurface oxygen and surface oxide formation at Ag(111): A density-functional theory investigation. *Physical Review B*, **2003**, 67,	3.3	127
2	Oxygen adsorption on Ag(111): A density-functional theory investigation. *Physical Review B*, **2002**, 65,	3.3	231
1	Synthesis of Iron-Carbide Nanoparticles: Identification of the Active Phase and Mechanism of Fe-Based Fischer-Tropsch Synthesis. *CCS Chemistry*,2712-2724	7.2	18