Wei-Xue Li

List of Publications by Year
in descending order

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127 papers	11,077 citations	41323 49 h-index	30058 103 g-index
130 all docs	130 docs citations	130 times ranked	11822 citing authors

#	Article	IF	Citations
1	Toward N-Doped Graphene via Solvothermal Synthesis. Chemistry of Materials, 2011, 23, 1188-1193.	3.2	984
2	Interface-Confined Ferrous Centers for Catalytic Oxidation. Science, 2010, 328, 1141-1144.	6.0	866
3	Engineering the electronic structure of single atom Ru sites via compressive strain boosts acidic water oxidation electrocatalysis. Nature Catalysis, 2019, 2, 304-313.	16.1	757
4	In-situ structure and catalytic mechanism of NiFe and CoFe layered double hydroxides during oxygen evolution. Nature Communications, 2020, 11, 2522.	5.8	594
5	Water-Mediated Marsâ€“Van Krevelen Mechanism for CO Oxidation on Ceria-Supported Single-Atom Pt₁ Catalyst. ACS Catalysis, 2017, 7, 887-891.	5.5	407
6	Atomistic Theory of Ostwald Ripening and Disintegration of Supported Metal Particles under Reaction Conditions. Journal of the American Chemical Society, 2013, 135, 1760-1771.	6.6	352
7	Crystallographic Dependence of CO Activation on Cobalt Catalysts: HCP versus FCC. Journal of the American Chemical Society, 2013, 135, 16284-16287.	6.6	348
8	Oxygen adsorption on Ag(111): A density-functional theory investigation. Physical Review B, 2002, 65, .	1.1	256
9	Sabatier principle of metal-support interaction for design of ultrastable metal nanocatalysts. Science, 2021, 374, 1360-1365.	6.0	250
10	High Alcohols Synthesis via Fischerâ€“Tropsch Reaction at Cobalt Metal/Carbide Interface. ACS Catalysis, 2015, 5, 3620-3624.	5.5	231
11	Supported Single Pt₁/Au₁ Atoms for Methanol Steam Reforming. ACS Catalysis, 2014, 4, 3886-3890.	5.5	204
12	Disentangling the size-dependent geometric and electronic effects of palladium nanocatalysts beyond selectivity. Science Advances, 2019, 5, eaat6413.	4.7	187
13	Crystalâ€Planeâ€Controlled Selectivity of Cu₂O Catalysts in Propylene Oxidation with Molecular Oxygen. Angewandte Chemie - International Edition, 2014, 53, 4856-4861.	7.2	180
14	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.	2.9	178
15	Insights into the function of silver as an oxidation catalyst byab initioatomistic thermodynamics. Physical Review B, 2003, 68, .	1.1	178
16	Intrinsic Electrocatalytic Activity for Oxygen Evolution of Crystalline 3dâ€Transition Metal Layered Double Hydroxides. Angewandte Chemie - International Edition, 2021, 60, 14446-14457.	7.2	170
17	Synergizing metalâ€“support interactions and spatial confinement boosts dynamics of atomic nickel for hydrogenations. Nature Nanotechnology, 2021, 16, 1141-1149.	15.6	165
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.	1.5	160

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19	Phaseâ€Selective Syntheses of Cobalt Telluride Nanofleeces for Efficient Oxygen Evolution Catalysts. Angewandte Chemie - International Edition, 2017, 56, 7769-7773.	7.2	157
20	Chemical Insights into the Design and Development of Face-Centered Cubic Ruthenium Catalysts for Fischerâ€“Tropsch Synthesis. Journal of the American Chemical Society, 2017, 139, 2267-2276.	6.6	147
21	The most active Cu facet for low-temperature water gas shift reaction. Nature Communications, 2017, 8, 488.	5.8	141
22	Size-Selective Carbon Nanoclusters as Precursors to the Growth of Epitaxial Graphene. Nano Letters, 2011, 11, 424-430.	4.5	139
23	Water enables mild oxidation of methane to methanol on gold single-atom catalysts. Nature Communications, 2021, 12, 1218.	5.8	138
24	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.	1.5	137
25	Subsurface oxygen and surface oxide formation at Ag(111): A density-functional theory investigation. Physical Review B, 2003, 67, .	1.1	135
26	Experimental observation of quantum oscillation of surface chemical reactivities. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 9204-9208.	3.3	123
27	In Situ Oxidation Study of Pt(110) and Its Interaction with CO. Journal of the American Chemical Society, 2011, 133, 20319-20325.	6.6	120
28	Platinum-Modulated Cobalt Nanocatalysts for Low-Temperature Aqueous-Phase Fischerâ€“Tropsch Synthesis. Journal of the American Chemical Society, 2013, 135, 4149-4158.	6.6	116
29	Growth of Single- and Bilayer ZnO on Au(111) and Interaction with Copper. Journal of Physical Chemistry C, 2013, 117, 11211-11218.	1.5	108
30	Carbon Chain Growth by Formyl Insertion on Rhodium and Cobalt Catalysts in Syngas Conversion. Angewandte Chemie - International Edition, 2011, 50, 5335-5338.	7.2	105
31	Bimetallic monolayer catalyst breaks the activityâ€“selectivity trade-off on metal particle size for efficient chemoselective hydrogenations. Nature Catalysis, 2021, 4, 840-849.	16.1	102
32	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.	6.6	99
33	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.	1.5	98
34	Hydrolysis of ball milling Alâ€“Biâ€“hydride and Alâ€“Biâ€“salt mixture for hydrogen generation. Journal of Alloys and Compounds, 2008, 460, 125-129.	2.8	93
35	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.	6.6	93
36	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, 11572-11579.	6.6	90

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37	Structural and electronic properties of cobalt carbide Co2C and its surface stability: Density functional theory study. Surface Science, 2012, 606, 598-604.	0.8	79
38	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.	1.5	73
39	Structure sensitivity of CO methanation on Co (0001), and surfaces: Density functional theory calculations. Catalysis Today, 2013, 215, 36-42.	2.2	72
40	Reversible Structural Modulation of Feâ€“Pt Bimetallic Surfaces and Its Effect on Reactivity. ChemPhysChem, 2009, 10, 1013-1016.	1.0	68
41	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.	1.5	64
42	Theory of nitride oxide adsorption on transition metal (111) surfaces: a first-principles investigation. Physical Chemistry Chemical Physics, 2010, 12, 2459.	1.3	63
43	Force reversed method for locating transition states. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	63
44	Rh-Decorated Cu Alloy Catalyst for Improved C₂Oxygenate Formation from Syngas. Journal of Physical Chemistry C, 2011, 115, 18247-18256.	1.5	62
45	Quantification of critical particle distance for mitigating catalyst sintering. Nature Communications, 2021, 12, 4865.	5.8	62
46	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.	1.5	59
47	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.	5.5	59
48	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.	1.5	56
49	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.	1.5	52
50	First Principle Study of Ethanol Adsorption and Formation of Hydrogen Bond on Rh(111) Surface. Journal of Physical Chemistry C, 2007, 111, 7403-7410.	1.5	50
51	Surface and interface design for heterogeneous catalysis. Physical Chemistry Chemical Physics, 2019, 21, 523-536.	1.3	49
52	Surface Iron Species in Palladiumâ€“Iron Intermetallic Nanocrystals that Promote and Stabilize CO₂ Methanation. Angewandte Chemie - International Edition, 2020, 59, 14434-14442.	7.2	49
53	Carbon Monoxide Activation on Cobalt Carbide for Fischerâ€“Tropsch Synthesis from First-Principles Theory. ACS Catalysis, 2019, 9, 8093-8103.	5.5	47
54	Modulating the reactivity of Ni-containing Pt(111)-skin catalysts by density functional theory calculations. Journal of Chemical Physics, 2008, 128, 194707.	1.2	46

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55	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, .	1.1	45
56	Establishing and Understanding Adsorptionâ€“Energy Scaling Relations with Negative Slopes. Journal of Physical Chemistry Letters, 2016, 7, 5302-5306.	2.1	43
57	First-Principles Investigation of Surface and Subsurface H Adsorption on Ir(111). Journal of Physical Chemistry C, 2009, 113, 21361-21367.	1.5	42
58	Surface Iron Species in Palladiumâ€“Iron Intermetallic Nanocrystals that Promote and Stabilize CO₂ Methanation. Angewandte Chemie, 2020, 132, 14542-14550.	1.6	41
59	Atomically dispersed Ir/Î±-MoC catalyst with high metal loading and thermal stability for water-promoted hydrogenation reaction. National Science Review, 2022, 9, nwab026.	4.6	41
60	Synthesis of Iron-Carbide Nanoparticles: Identification of the Active Phase and Mechanism of Fe-Based Fischerâ€“Tropsch Synthesis. CCS Chemistry, 2021, 3, 2712-2724.	4.6	41
61	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.	3.6	37
62	Direct Imaging Single Methanol Molecule Photocatalysis on Titania. Journal of Physical Chemistry C, 2015, 119, 17748-17754.	1.5	37
63	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.	1.5	37
64	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.	1.5	37
65	Theoretical study of crystal phase effect in heterogeneous catalysis. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 571-583.	6.2	36
66	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.	1.5	35
67	In Situ Spectroscopic Characterization and Theoretical Calculations Identify Partially Reduced ZnO_{1â^'x}/Cu Interfaces for Methanol Synthesis from CO₂. Angewandte Chemie - International Edition, 2022, 61, .	7.2	34
68	The improved electrochemical properties of novel Laâ€“Mgâ€“Ni-based hydrogen storage composites. Electrochimica Acta, 2007, 52, 6700-6706.	2.6	33
69	First-principles study of hydrogen absorption on Mg(0001) and formation of magnesium hydride. Physical Review B, 2010, 81, .	1.1	33
70	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.	2.2	33
71	In- and Out-Dependent Interactions of Iron with Carbon Nanotubes. Journal of Physical Chemistry C, 2012, 116, 16461-16466.	1.5	30
72	First-principles study of structure sensitivity of chain growth and selectivity in Fischerâ€“Tropsch synthesis using HCP cobalt catalysts. Catalysis Science and Technology, 2017, 7, 2967-2977.	2.1	30

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73	Intrinsic Electrocatalytic Activity for Oxygen Evolution of Crystalline 3dâ€Transition Metal Layered Double Hydroxides. Angewandte Chemie, 2021, 133, 14567-14578.	1.6	30
74	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.	1.5	27
75	First-principles study of single transition metal atoms on ZnO for the water gas shift reaction. Catalysis Science and Technology, 2017, 7, 4294-4301.	2.1	27
76	Carbon monoxide adsorption and dissociation on Mn-decorated Rh(111) and Rh(553) surfaces: A first-principles study. Catalysis Today, 2011, 160, 228-233.	2.2	26
77	Influence of Particle Size Distribution on Lifetime and Thermal Stability of Ostwald Ripening of Supported Particles. ChemCatChem, 2018, 10, 2900-2907.	1.8	26
78	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.	1.5	26
79	Unique Reactivity of Confined Metal Atoms on a Silicon Substrate. ChemPhysChem, 2008, 9, 975-979.	1.0	24
80	Reconstruction of the Wet Chemical Synthesis Process: The Case of Fe₅C₂ Nanoparticles. Journal of Physical Chemistry C, 2017, 121, 5154-5160.	1.5	24
81	Step enhanced dehydrogenation of ethanol on Rh. Surface Science, 2008, 602, 3057-3063.	0.8	23
82	Cooperative activation in ring-opening hydrolysis of epoxides by Co-salen complexes: A first principle study. Chemical Physics Letters, 2009, 470, 259-263.	1.2	20
83	First-principles study of the adsorption of Au atoms and Au<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>and Au<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>clusters on FeO/Pt(111). Physical Review B, 2011, 84, .	1.1	20
84	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.	1.5	20
85	Interplay Between Site Activity and Density of BCC Iron for Ammonia Synthesis Based on Firstâ€Principles Theory. ChemCatChem, 2019, 11, 1928-1934.	1.8	20
86	Nitrogen-doped graphene layers for electrochemical oxygen reduction reaction boosted by lattice strain. Journal of Catalysis, 2019, 378, 113-120.	3.1	19
87	Influence of Cobalt Crystal Structures on Activation of Nitrogen Molecule: A First-Principles Study. Journal of Physical Chemistry C, 2019, 123, 10956-10966.	1.5	19
88	First-Principles Kinetic Study for Ostwald Ripening of Late Transition Metals on TiO₂(110). Journal of Physical Chemistry C, 2019, 123, 1160-1169.	1.5	19
89	Density functional theory study of CHx (x=1â€“3) adsorption on clean and CO precovered Rh(111) surfaces. Journal of Chemical Physics, 2007, 127, 024705.	1.2	18
90	Wavevector-dependent quantum-size effect in electron decay length at Pb thin film surfaces. Applied Physics Letters, 2008, 93, 093105.	1.5	18

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91	Carbon induced selective regulation of cobalt-based Fischerâ€“Tropsch catalysts by ethylene treatment. Faraday Discussions, 2017, 197, 207-224.	1.6	17
92	Density functional theory andab initiomolecular dynamics study of NO adsorption on Pd(111) and Pt(111) surfaces. Physical Review B, 2010, 81, .	1.1	16
93	Theoretical Investigation of Metalâ€Support Interactions on Ripening Kinetics of Supported Particles. ChemNanoMat, 2018, 4, 510-517.	1.5	16
94	Atomic and molecular adsorption on RhMn alloy surface: A first principles study. Journal of Chemical Physics, 2008, 129, 244711.	1.2	13
95	Oxidation of platinum surfaces and reaction with carbon monoxide. Journal of Physics Condensed Matter, 2008, 20, 184022.	0.7	13
96	A Firstâ€Principles Study of Carbonâ€“Oxygen Bond Scission in Multiatomic Molecules on Flat and Stepped Metal Surfaces. ChemCatChem, 2014, 6, 1755-1762.	1.8	13
97	First-Principles microkinetic study of methanol synthesis on Cu(221) and ZnCu(221) surfaces. Chinese Journal of Chemical Physics, 2018, 31, 284-290.	0.6	13
98	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.	1.5	13
99	Adsorption Features of Formaldehyde on TiO₂(110) Surface Probed by High-Resolution Scanning Tunnelling Microscopy. Journal of Physical Chemistry Letters, 2019, 10, 3352-3358.	2.1	13
100	Hydroxyl improving the activity, selectivity and stability of supported Ni single atoms for selective semi-hydrogenation. Chemical Science, 2021, 12, 10290-10298.	3.7	13
101	H₂ Activation on Pristine and Substitutional ZnO(101Ì…0) and Cr₂O₃(001) Surfaces by Density Functional Theory Calculations. Journal of Physical Chemistry C, 2022, 126, 9059-9068.	1.5	13
102	A first-principles study on the behavior of HCl inside SWCNT. Computational and Theoretical Chemistry, 2009, 905, 44-47.	1.5	12
103	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.	7.1	12
104	Bridge sulfur vacancies in MoS2 catalyst for reverse water gas shift: A first-principles study. Applied Surface Science, 2021, 561, 149925.	3.1	12
105	First-principles study of water activation on Cu-ZnO catalysts. Chinese Journal of Catalysis, 2013, 34, 1705-1711.	6.9	11
106	Metal-support interaction controlled migration and coalescence of supported particles. Science China Technological Sciences, 2019, 62, 762-772.	2.0	11
107	K-Edge XANES Investigation of Fe-Based Oxides by Density Functional Theory Calculations. Journal of Physical Chemistry C, 2021, 125, 26229-26239.	1.5	11
108	Stability of polar ZnO surfaces studied by pair potential method and local energy density method. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	10

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109	First-principles investigation of electrochemical dissolution of Pt nanoparticles and kinetic simulation. Journal of Chemical Physics, 2019, 151, 234711.	1.2	10
110	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.	1.5	10
111	Probing surface defects of ZnO using formaldehyde. Journal of Chemical Physics, 2020, 152, 074714.	1.2	10
112	Machine-learning adsorption on binary alloy surfaces for catalyst screening. Chinese Journal of Chemical Physics, 2020, 33, 703-711.	0.6	9
113	Understanding Surface Catalyzed Decomposition Reactions Using a Chemical Pathway Analysis. Journal of Physical Chemistry C, 2018, 122, 28158-28172.	1.5	8
114	Bimetallic Cu/Rh Catalyst for Preferential Oxidation of CO in H₂: a DFT Study. Journal of Physical Chemistry C, 2021, 125, 19697-19705.	1.5	7
115	In Situ Spectroscopic Characterization and Theoretical Calculations Identify Partially Reduced ZnO_{1â”x}/Cu Interfaces for Methanol Synthesis from CO₂. Angewandte Chemie, 2022, 134, .	1.6	6
116	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.	2.1	5
117	Finding Key Factors for Efficient Water and Methanol Activation at Metals, Oxides, MXenes, and Metal/Oxide Interfaces. ACS Catalysis, 2022, 12, 1237-1246.	5.5	5
118	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.	0.5	4
119	Ligand Stabilized Ni 1 Catalyst for Efficient CO Oxidation. ChemPhysChem, 2020, 21, 2417-2425.	1.0	4
120	Crystallographic and morphological sensitivity of N2 activation over ruthenium. Chinese Journal of Chemical Physics, 2021, 34, 263-272.	0.6	4
121	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.	6.9	3
122	Dynamic chemical processes on ZnO surfaces tuned by physisorption under ambient conditions. Journal of Energy Chemistry, 2022, , .	7.1	3
123	Influence of nickel(II) oxide surface magnetism on molecule adsorption: A first-principles study. Chinese Journal of Catalysis, 2017, 38, 1736-1748.	6.9	2
124	Band structure and Fermi surface of atomically uniform lead films. New Journal of Physics, 2010, 12, 113034.	1.2	1
125	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.	1.5	1
126	Frontispiece: Surface Iron Species in Palladiumâ€“Iron Intermetallic Nanocrystals that Promote and Stabilize CO₂ Methanation. Angewandte Chemie - International Edition, 2020, 59, .	7.2	0

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127	Frontispiz: Surface Iron Species in Palladiumâ€“Iron Intermetallic Nanocrystals that Promote and Stabilize CO₂ Methanation. Angewandte Chemie, 2020, 132, .	1.6	0