

# Xiao-Dong Wen

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

369  
papers

23,075  
citations

77  
h-index

145  
g-index

391  
ext. papers

29,043  
ext. citations

9.5  
avg, IF

7.17  
L-index

#	Paper	IF	Citations
369	Atomistic insights of a chemical complexity effect on the irradiation resistance of high entropy alloys. <i>Materials Advances</i> , <b>2022</b> , 3, 1680-1686	3.3	1
368	Theoretical insight into the interaction between hydrogen and Hg carbide (Fe <sub>5</sub> C <sub>2</sub> ) surfaces. <i>Applied Surface Science</i> , <b>2022</b> , 583, 152538	6.7	0
367	A Molecular Dynamics Study of the Stability and Mechanical Properties of a Nano-Engineered Fuzzy Carbon Fiber Composite. <i>Journal of Composites Science</i> , <b>2022</b> , 6, 54	3	
366	Distinct Crystal-Facet-Dependent Behaviors for Single-Atom Palladium-on-Ceria Catalysts: Enhanced Stabilization and Catalytic Properties.. <i>Advanced Materials</i> , <b>2022</b> , e2107721	24	4
365	Genesis of an Fe <sub>5</sub> C <sub>2</sub> @Fe <sub>3</sub> O <sub>4</sub> core/shell structure during CO carburization of metallic iron nanoparticles. <i>Journal of Catalysis</i> , <b>2022</b> , 407, 97-103	7.3	2
364	Fe-Sn bimetallic catalysts for an enhanced Fischer-Tropsch synthesis stability via oxygen removal and coking resistance. <i>Fuel</i> , <b>2022</b> , 311, 122115	7.1	0
363	Defect-rich graphene stabilized atomically dispersed Cu <sub>3</sub> clusters with enhanced oxidase-like activity for antibacterial applications. <i>Applied Catalysis B: Environmental</i> , <b>2022</b> , 301, 120826	21.8	6
362	Dissociative adsorption of H <sub>2</sub> O and CO <sub>2</sub> on the clean and O-pre-covered high index Ru surfaces: Corrugated Ru(110 $\bar{1}$ ) and stepped Ru(200 $\bar{1}$ ) surfaces. <i>Surface Science</i> , <b>2022</b> , 715, 121936	1.8	0
361	Engineering Lattice Disorder on a Photocatalyst: Photochromic BiOBr Nanosheets Enhance Activation of Aromatic C-H Bonds via Water Oxidation.. <i>Journal of the American Chemical Society</i> , <b>2022</b> ,	16.4	11
360	Mechanical Properties and Buckling of Kagome Graphene under Tension: A Molecular Dynamics Study. <i>Crystals</i> , <b>2022</b> , 12, 292	2.3	1
359	Visualization of on-surface ethylene polymerization through ethylene insertion.. <i>Science</i> , <b>2022</b> , 375, 1188-1191	319.2	
358	Pressure-Induced Amorphization and Crystallization of Heterophase Pd Nanostructures.. <i>Small</i> , <b>2022</b> , e2106396	11	0
357	First-Principles Study of Three-Dimensional Electrides Containing One-Dimensional [BaN] Chains.. <i>ACS Omega</i> , <b>2022</b> , 7, 13290-13298	3.9	
356	Theoretical study about adsorbed oxygen reduction over Fe <sub>5</sub> C <sub>2</sub> : formation of H <sub>2</sub> O and CO <sub>2</sub> . <i>Molecular Catalysis</i> , <b>2022</b> , 524, 112236	3.3	
355	Insight into the Activity of Atomically Dispersed Cu Catalysts for Semihydrogenation of Acetylene: Impact of Coordination Environments. <i>ACS Catalysis</i> , <b>2022</b> , 12, 48-57	13.1	3
354	Surface Hydroxyl Dependent Adsorption of Ruthenium on SiO <sub>2</sub> (001) - Understanding MetalSupport Interaction. <i>Applied Surface Science</i> , <b>2022</b> , 153396	6.7	0
353	Elucidating the effect of sodium on the carburization behaviors of Fe under CO or C <sub>2</sub> H <sub>4</sub> . <i>Applied Catalysis B: Environmental</i> , <b>2022</b> , 315, 121527	21.8	1

352	C2 weakens the turnover frequency during the melting of Fe <sub>3</sub> Cy: insights from reactive MD simulations. <i>New Journal of Chemistry</i> , <b>2021</b> , 46, 282-293	3.6	
351	The Crack Angle of 60° Is the Most Vulnerable Crack Front in Graphene According to MD Simulations. <i>Crystals</i> , <b>2021</b> , 11, 1355	2.3	3
350	First-principles study on the mechanism of water-gas shift reaction on the Fe <sub>3</sub> O <sub>4</sub> (111)-Fe <sub>2</sub> O <sub>3</sub> . <i>Molecular Catalysis</i> , <b>2021</b> , 516, 111998	3.3	1
349	Reversing sintering effect of Ni particles on γ-MoN via strong metal support interaction. <i>Nature Communications</i> , <b>2021</b> , 12, 6978	17.4	5
348	Cobalt Single Atom Incorporated in Ruthenium Oxide Sphere: A Robust Bifunctional Electrocatalyst for HER and OER. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> ,	16.4	16
347	A combined DFTB nanoreactor and reaction network generator approach for the mechanism of hydrocarbon combustion. <i>Chemical Communications</i> , <b>2021</b> , 57, 11633-11636	5.8	2
346	Tuning the selectivity of catalytic nitriles hydrogenation by structure regulation in atomically dispersed Pd catalysts. <i>Nature Communications</i> , <b>2021</b> , 12, 6194	17.4	11
345	Atomic Insights into Fracture Characteristics of Twisted Tri-Layer Graphene. <i>Crystals</i> , <b>2021</b> , 11, 1202	2.3	4
344	Simple mechanisms of CH <sub>4</sub> reforming with CO and H <sub>2</sub> O on a supported Ni/ZrO <sub>2</sub> catalyst. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 26392-26400	3.6	0
343	Atomically Dispersed Ni/γ-MoC Catalyst for Hydrogen Production from Methanol/Water. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 309-317	16.4	60
342	Nonoxidative Conversion of Methane, Ethane, and Ethylene on Flat Ir(111) and Stepped Ir(211) Surfaces. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 5602-5615	3.8	1
341	Intrinsic mechanism of active metal dependent primary amine selectivity in the reductive amination of carbonyl compounds. <i>Journal of Catalysis</i> , <b>2021</b> , 395, 293-301	7.3	5
340	The role of ligands in pressure-induced phase transition of gold nanoribbons. <i>Phase Transitions</i> , <b>2021</b> , 94, 123-133	1.3	0
339	Impact of Polypyrrole Functionalization on the Anodic Performance of Boron Nitride Nanosheets: Insights From First-Principles Calculations. <i>Frontiers in Chemistry</i> , <b>2021</b> , 9, 670833	5	5
338	Regulating coordination number in atomically dispersed Pt species on defect-rich graphene for n-butane dehydrogenation reaction. <i>Nature Communications</i> , <b>2021</b> , 12, 2664	17.4	44
337	Atomic Co/Ni dual sites with N/P-coordination as bifunctional oxygen electrocatalyst for rechargeable zinc-air batteries. <i>Nano Research</i> , <b>2021</b> , 14, 3482-3488	10	27
336	Fragility under shocking: molecular dynamics insights into defect evolutions in tungsten lattice. <i>Tungsten</i> , <b>2021</b> , 3, 234-242	4.6	4
335	Ab Initio Investigation of Helium Mobility in La <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> Pyrochlore. <i>Crystals</i> , <b>2021</b> , 11, 667	2.3	1

334	New insight into seeding process leading to improved zeolitic acidity and surface properties for its catalytic application in propane aromatization. <i>Catalysis Today</i> , <b>2021</b> , 368, 232-242	5.3	5
333	Comprehensive understanding of SiO <sub>2</sub> -promoted Fe Fischer-Tropsch synthesis catalysts: Fe-SiO <sub>2</sub> interaction and beyond. <i>Catalysis Today</i> , <b>2021</b> , 368, 96-105	5.3	7
332	Interactive network of the dehydrogenation of alkanes, alkenes and alkynes & surface carbon hydrogenative coupling on Ru(111). <i>Catalysis Science and Technology</i> , <b>2021</b> , 11, 191-210	5.5	2
331	Porous Fe <sub>2</sub> O <sub>3</sub> nanoparticle decorated with atomically dispersed platinum: Study on atomic site structural change and gas sensor activity evolution. <i>Nano Research</i> , <b>2021</b> , 14, 1435-1442	10	17
330	Reduced Plastic Dilatancy in Polymer Glasses. <i>Macromolecular Theory and Simulations</i> , <b>2021</b> , 30, 2000063	1.5	1
329	Selective regulation of n-dodecane isomerization and cracking performance in Pt/beta catalysts via orientation control of Brønsted acid site distribution. <i>Catalysis Science and Technology</i> , <b>2021</b> , 11, 2094-2102	5.5	0
328	Manganese vacancy-confined single-atom Ag in cryptomelane nanorods for efficient Wacker oxidation of styrene derivatives. <i>Chemical Science</i> , <b>2021</b> , 12, 6099-6106	9.4	8
327	Performance of SCAN Meta-GGA Functionals on Nonlinear Mechanics of Graphene-Like g-SiC. <i>Crystals</i> , <b>2021</b> , 11, 120	2.3	
326	Mapping surface morphology and phase evolution of iron sulfide nanoparticles. <i>CrystEngComm</i> , <b>2021</b> , 23, 5645-5654	3.3	1
325	Prediction Of Material Properties By Neural Network Fusing The Atomic Local Environment And Global Description: Applied To Organic Molecules And Crystals. <i>E3S Web of Conferences</i> , <b>2021</b> , 267, 02059	0.5	0
324	Fe <sub>1</sub> N <sub>4</sub> D <sub>1</sub> site with axial Fe <sub>D</sub> coordination for highly selective CO <sub>2</sub> reduction over a wide potential range. <i>Energy and Environmental Science</i> , <b>2021</b> , 14, 3430-3437	35.4	40
323	A stable low-temperature H <sub>2</sub> -production catalyst by crowding Pt on FeMoC. <i>Nature</i> , <b>2021</b> , 589, 396-401	50.4	109
322	Ultrahigh Ballistic Resistance of Twisted Bilayer Graphene. <i>Crystals</i> , <b>2021</b> , 11, 206	2.3	5
321	Theoretical Perspectives on the Modulation of Carbon on Transition-Metal Catalysts for Conversion of Carbon-Containing Resources. <i>ACS Catalysis</i> , <b>2021</b> , 11, 2156-2181	13.1	9
320	Fe-Based Catalysts for the Direct Photohydrogenation of CO <sub>2</sub> to Value-Added Hydrocarbons. <i>Advanced Energy Materials</i> , <b>2021</b> , 11, 2002783	21.8	35
319	Glucose-Induced Monodisperse Iron Oxide/Graphene Oxide Catalysts for Efficient Fischer-Tropsch Synthesis. <i>Energy &amp; Fuels</i> , <b>2021</b> , 35, 4428-4436	4.1	1
318	Carbon Deposition and Permeation on Nickel Surfaces in Operando Conditions: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 7166-7177	3.8	3
317	Rationally Designed Metal Cocatalyst for Selective Photosynthesis of Bibenzyls via Dehalogenative C-C Homocoupling. <i>ACS Catalysis</i> , <b>2021</b> , 11, 4338-4348	13.1	8

3 <sup>16</sup>	Stretchable and Anisotropic Conductive Composite Hydrogel as Therapeutic Cardiac Patches <b>2021</b> , 3, 1238-1248		6
3 <sup>15</sup>	Titania-Supported Ni P/Ni Catalysts for Selective Solar-Driven CO Hydrogenation. <i>Advanced Materials</i> , <b>2021</b> , 33, e2103248	24	12
3 <sup>14</sup>	Mechanisms of Double-Bond Isomerization Reactions of n-Butene on Different Lewis Acids. <i>ACS Catalysis</i> , <b>2021</b> , 11, 11293-11304	13.1	3
3 <sup>13</sup>	Anion-exchange-mediated internal electric field for boosting photogenerated carrier separation and utilization. <i>Nature Communications</i> , <b>2021</b> , 12, 4952	17.4	12
3 <sup>12</sup>	The Facile Dissociation of Carbon-Oxygen Bonds in CO and CO on the Surface of LaCoSiH Intermetallic Compound. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 25538-25545	16.4	1
3 <sup>11</sup>	The Facile Dissociation of Carbon-Oxygen Bonds in CO <sub>2</sub> and CO on the Surface of LaCoSiH <sub>x</sub> Intermetallic Compound. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 25742	3.6	
3 <sup>10</sup>	Insights into Coke Formation and Removal under Operating Conditions with a Quantum Nanoreactor Approach. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 9413-9421	6.4	1
3 <sup>09</sup>	Low-Temperature Hydrogenation of Toluene Using an Iron-Promoted Molybdenum Carbide Catalyst. <i>Catalysts</i> , <b>2021</b> , 11, 1079	4	
3 <sup>08</sup>	Cooperative Sites in Fully Exposed Pd Clusters for Low-Temperature Direct Dehydrogenation Reaction. <i>ACS Catalysis</i> , <b>2021</b> , 11, 11469-11477	13.1	12
3 <sup>07</sup>	Role of Interfaces in the Thermal Reduction Process of the FeO/Cu <sub>2</sub> O/Cu(100) Surface. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 20863-20869	3.8	1
3 <sup>06</sup>	The effect of surface carbon on ethylene dimerization. <i>Applied Surface Science</i> , <b>2021</b> , 570, 151210	6.7	1
3 <sup>05</sup>	Wet-chemistry approach for the synthesis of single phase ferromagnetic Co <sub>3</sub> C nanoparticle. <i>Nano Select</i> , <b>2021</b> , 2, 1368-1371	3.1	1
3 <sup>04</sup>	Oxygen Adsorption-Induced Morphological Evolution of H <sub>11</sub> g Iron Carbide at High Oxygen Chemical Potentials. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 3055-3065	3.8	1
3 <sup>03</sup>	Highly Selective Aromatization of Octane over Pt-Zn/UZSM-5: The Effect of Pt-Zn Interaction and Pt Position. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2020</b> , 12, 28273-28287	9.5	10
3 <sup>02</sup>	The structural information filtered features (SIFF) potential: Maximizing information stored in machine-learning descriptors for materials prediction. <i>Journal of Applied Physics</i> , <b>2020</b> , 127, 215108	2.5	1
3 <sup>01</sup>	Iridium single-atom catalyst on nitrogen-doped carbon for formic acid oxidation synthesized using a general host-guest strategy. <i>Nature Chemistry</i> , <b>2020</b> , 12, 764-772	17.6	207
3 <sup>00</sup>	Mesoporous Iron Oxide Nanoparticle-Decorated Graphene Oxide Catalysts for Fischer-Tropsch Synthesis. <i>ACS Applied Nano Materials</i> , <b>2020</b> , 3, 7182-7191	5.6	13
2 <sup>99</sup>	Exploring direct and hydrogen-assisted CO activation on iridium surfaces: Surface dependent activity. <i>Catalysis Science and Technology</i> , <b>2020</b> , 10, 4424-4435	5.5	2

298	Fabricating Pd isolated single atom sites on C <sub>3</sub> N <sub>4</sub> /rGO for heterogenization of homogeneous catalysis. <i>Nano Research</i> , <b>2020</b> , 13, 947-951	10	41
297	Single-atom Rh/N-doped carbon electrocatalyst for formic acid oxidation. <i>Nature Nanotechnology</i> , <b>2020</b> , 15, 390-397	28.7	208
296	Atomic site electrocatalysts for water splitting, oxygen reduction and selective oxidation. <i>Chemical Society Reviews</i> , <b>2020</b> , 49, 2215-2264	58.5	309
295	Predicting Crystal Morphology Using a Geometric Descriptor: A Comparative Study of Elemental Crystals with High-Throughput DFT Calculations. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 15920-15927	7.8	3
294	Fabrication of a core-shell MFI@TON material and its enhanced catalytic performance for toluene alkylation. <i>Catalysis Science and Technology</i> , <b>2020</b> , 10, 1281-1291	5.5	3
293	Adsorption and Diffusion of Hydrogen in Carbon Honeycomb. <i>Nanomaterials</i> , <b>2020</b> , 10,	5.4	8
292	Preparation of electron-rich Fe-based catalyst via electronic structure regulation and its promotion to hydrodesulfurization of dibenzothiophene. <i>Applied Catalysis B: Environmental</i> , <b>2020</b> , 269, 118779	21.8	7
291	MOF derived high-density atomic platinum heterogeneous catalyst for C≡ bond activation. <i>Materials Chemistry Frontiers</i> , <b>2020</b> , 4, 1158-1163	7.8	4
290	Electronic effects of transition metal dopants on Fe(100) and Fe <sub>5</sub> C <sub>2</sub> (100) surfaces for CO activation. <i>Catalysis Science and Technology</i> , <b>2020</b> , 10, 2047-2056	5.5	5
289	Tuning Polarity of Cu-O Bond in Heterogeneous Cu Catalyst to Promote Additive-free Hydroboration of Alkynes. <i>Chem</i> , <b>2020</b> , 6, 725-737	16.2	53
288	Relationship between the Behavior of Hydrogen and Hydrogen Bubble Nucleation in Vanadium. <i>Materials</i> , <b>2020</b> , 13,	3.5	2
287	Hydrodeoxygenation of anisole to benzene over an Fe <sub>2</sub> P catalyst by a direct deoxygenation pathway. <i>Catalysis Science and Technology</i> , <b>2020</b> , 10, 3015-3023	5.5	10
286	Highly Efficient Polarized GeS/MoSe <sub>2</sub> van der Waals Heterostructure for Water Splitting from Ultraviolet to Near-Infrared Light. <i>Physica Status Solidi - Rapid Research Letters</i> , <b>2020</b> , 14, 1900582	2.5	10
285	Hydrogen Adsorption on Ir(111), Ir(100) and Ir(110) Surface and Coverage Dependence. <i>Surface Science</i> , <b>2020</b> , 692, 121514	1.8	4
284	DFT study on H <sub>2</sub> and H adsorption and the electronic properties of single atom Cu modified Fe (1 1 1) surface. <i>Applied Surface Science</i> , <b>2020</b> , 505, 144526	6.7	3
283	Synergistically Interactive Pyridinic-N/MoP Sites: Identified Active Centers for Enhanced Hydrogen Evolution in Alkaline Solution. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 9067-9075	3.6	24
282	Insight into the magnetic moment of iron borides: theoretical consideration from the local coordinative and electronic environment. <i>Dalton Transactions</i> , <b>2020</b> , 49, 2168-2175	4.3	2
281	Mechanistic Aspects of CO Activation and C≡ Bond Formation on the Fe/C- and Fe-Terminated Fe <sub>3</sub> C(010) Surfaces. <i>ACS Catalysis</i> , <b>2020</b> , 10, 877-890	13.1	9

280	Suppressing Metal Leaching in a Supported Co/SiO <sub>2</sub> Catalyst with Effective Protectants in the Hydroformylation Reaction. <i>ACS Catalysis</i> , <b>2020</b> , 10, 914-920	13.1	25
279	Manganese Oxide Modified Nickel Catalysts for Photothermal CO Hydrogenation to Light Olefins. <i>Advanced Energy Materials</i> , <b>2020</b> , 10, 1902860	21.8	28
278	Nano-ZrO <sub>2</sub> as hydrogenation phase in bi-functional catalyst for syngas aromatization. <i>Fuel</i> , <b>2020</b> , 263, 116803	7.1	7
277	Impact of the Coordination Environment on Atomically Dispersed Pt Catalysts for Oxygen Reduction Reaction. <i>ACS Catalysis</i> , <b>2020</b> , 10, 907-913	13.1	68
276	Temperature-dependent surface free energy and the Wulff shape of iron and iron carbide nanoparticles: A molecular dynamics study. <i>Applied Surface Science</i> , <b>2020</b> , 509, 144859	6.7	8
275	Solving Chemistry Problems via an End-to-End Approach: A Proof of Concept. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 8866-8873	2.8	5
274	Theoretical exploration of intrinsic facet-dependent CH <sub>4</sub> and C <sub>2</sub> formation on Fe <sub>5</sub> C <sub>2</sub> particle. <i>Applied Catalysis B: Environmental</i> , <b>2020</b> , 278, 119308	21.8	13
273	Inverse ZrO/Cu as a highly efficient methanol synthesis catalyst from CO hydrogenation. <i>Nature Communications</i> , <b>2020</b> , 11, 5767	17.4	51
272	Coverage-Dependent Water Dissociative Adsorption Properties on Nickel Surfaces. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 25835-25845	3.8	4
271	Theoretical Insights into the Structure and Activity of Cobalt Modulated by Surface and Subsurface Carbon in Operando Conditions. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 18576-18586	3.8	2
270	Promotive effect of boron oxide on the iron-based catalysts for Fischer-Tropsch synthesis. <i>Fuel</i> , <b>2020</b> , 281, 118714	7.1	5
269	Crystal Structure Prediction Approach to Explore the Iron Carbide Phases: Novel Crystal Structures and Unexpected Magnetic Properties. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 17244-17254	3.8	4
268	The Application of Godunov SPH in the Simulation of Energetic Materials. <i>International Journal of Computational Methods</i> , <b>2020</b> , 17, 1950028	1.1	1
267	Isolated Single-Atom Ruthenium Anchored on Beta Zeolite as an Efficient Heterogeneous Catalyst for Styrene Epoxidation. <i>ChemNanoMat</i> , <b>2020</b> , 6, 1647-1651	3.5	3
266	Synergistically Interactive Pyridinic-N-MoP Sites: Identified Active Centers for Enhanced Hydrogen Evolution in Alkaline Solution. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 8982-8990	16.4	134
265	Adsorption or deoxidation of H <sub>2</sub> interacted with Fe <sub>3</sub> O <sub>4</sub> surface under different H coverage: A DFT study. <i>Applied Surface Science</i> , <b>2020</b> , 502, 144097	6.7	4
264	Efficient One-Pot Synthesis of Higher Alcohols from Syngas Catalyzed by Iron Nitrides. <i>ChemCatChem</i> , <b>2020</b> , 12, 1939-1943	5.2	4
263	Isolated Iron Single-Atomic Site-Catalyzed Chemoselective Transfer Hydrogenation of Nitroarenes to Arylamines. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 33819-33824	9.5	42

262	Investigation of the effects of phosphorus on the selective hydrodeoxygenation of anisole over an Fe/SiO <sub>2</sub> catalyst. <i>Catalysis Science and Technology</i> , <b>2019</b> , 9, 5712-5724	5.5	16
261	Predication of screened hybrid functional on transition metal monoxides: From Mott insulator to charge transfer insulator. <i>Journal of Alloys and Compounds</i> , <b>2019</b> , 808, 151707	5.7	1
260	Regulating the coordination structure of single-atom Fe-NC catalytic sites for benzene oxidation. <i>Nature Communications</i> , <b>2019</b> , 10, 4290	17.4	173
259	Anchoring Cu species over nanodiamond-graphene for semi-hydrogenation of acetylene. <i>Nature Communications</i> , <b>2019</b> , 10, 4431	17.4	118
258	Molecular or dissociative adsorption of water on clean and oxygen pre-covered Ni(111) surfaces. <i>Catalysis Science and Technology</i> , <b>2019</b> , 9, 199-212	5.5	6
257	Copper atom-pair catalyst anchored on alloy nanowires for selective and efficient electrochemical reduction of CO. <i>Nature Chemistry</i> , <b>2019</b> , 11, 222-228	17.6	337
256	Topological self-template directed synthesis of multi-shelled intermetallic NiGa hollow microspheres for the selective hydrogenation of alkyne. <i>Chemical Science</i> , <b>2019</b> , 10, 614-619	9.4	20
255	MXene (TiC) Vacancy-Confined Single-Atom Catalyst for Efficient Functionalization of CO. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 4086-4093	16.4	277
254	Mechanical Properties of Vacancy Tuned Carbon Honeycomb. <i>Nanomaterials</i> , <b>2019</b> , 9,	5.4	12
253	Carbon Permeation: The Prerequisite Elementary Step in Iron-Catalyzed Fischer-Tropsch Synthesis. <i>Catalysis Letters</i> , <b>2019</b> , 149, 645-664	2.8	13
252	Carbon Nanotubes Enhance the Radiation Resistance of bcc Iron Revealed by Atomistic Study. <i>Materials</i> , <b>2019</b> , 12,	3.5	6
251	Strain Enhanced Visible-Ultraviolet Absorption of Blue Phosphorene/MoX <sub>2</sub> (X = S,Se) Heterolayers. <i>Physica Status Solidi - Rapid Research Letters</i> , <b>2019</b> , 13, 1800659	2.5	5
250	A General Strategy for Fabricating Isolated Single Metal Atomic Site Catalysts in Y Zeolite. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 9305-9311	16.4	124
249	Mechanistic insight into CO activation, methanation and C-C bond formation from coverage dependent CO hydrogenation on Fe(110). <i>Surface Science</i> , <b>2019</b> , 689, 121456	1.8	7
248	Mechanism of Graphene Formation via Detonation Synthesis: A DFTB Nanoreactor Approach. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 3654-3665	6.4	13
247	The structure-activity relationship of Fe nanoparticles in CO adsorption and dissociation by reactive molecular dynamics simulations. <i>Journal of Catalysis</i> , <b>2019</b> , 374, 150-160	7.3	11
246	Effect of Angle, Temperature and Vacancy Defects on Mechanical Properties of PSI-Graphene. <i>Crystals</i> , <b>2019</b> , 9, 238	2.3	8
245	Convenient fabrication of BiOBr ultrathin nanosheets with rich oxygen vacancies for photocatalytic selective oxidation of secondary amines. <i>Nano Research</i> , <b>2019</b> , 12, 1625-1630	10	62



244	Nano-sized ZrO <sub>2</sub> derived from metal-organic frameworks and their catalytic performance for aromatic synthesis from syngas. <i>Catalysis Science and Technology</i> , <b>2019</b> , 9, 2982-2992	5.5	17
243	Exploration of Properties from Both the Bulk and Surface of Iron Silicides: A Unified Theoretical Study. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 11939-11949	3.8	3
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237	Tin-Assisted Fully Exposed Platinum Clusters Stabilized on Defect-Rich Graphene for Dehydrogenation Reaction. <i>ACS Catalysis</i> , <b>2019</b> , 9, 5998-6005	13.1	92
236	The Temperature-Sensitive Anisotropic Negative Poisson's Ratio of Carbon Honeycomb. <i>Nanomaterials</i> , <b>2019</b> , 9,	5.4	11
235	Recent Progress on Irradiation-Induced Defect Engineering of Two-Dimensional 2H-MoS <sub>2</sub> Few Layers. <i>Applied Sciences (Switzerland)</i> , <b>2019</b> , 9, 678	2.6	21
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227	Functionalization of Hollow Nanomaterials for Catalytic Applications: Nanoreactor Construction. <i>Advanced Materials</i> , <b>2019</b> , 31, e1800426	24	147

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110	Insight into the structure and energy of Mo <sub>27</sub> S <sub>x</sub> O <sub>y</sub> clusters. <i>RSC Advances</i> , <b>2017</b> , 7, 9513-9520	3.7	15
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106	Promotion of the Inactive Iron Sulfide to an Efficient Hydrodesulfurization Catalyst. <i>ACS Catalysis</i> , <b>2017</b> , 7, 4805-4816	13.1	43
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104	Application of the dimensional reduction formalism to PbBa[Li(PO)(PO)] (x = 0, 2, 6, 7): a series of phosphates with two types of isolated polyphosphate groups. <i>Dalton Transactions</i> , <b>2017</b> , 46, 4678-4684	4.3	11
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102	Rational Design of Single Molybdenum Atoms Anchored on N-Doped Carbon for Effective Hydrogen Evolution Reaction. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 16086-16090	16.4	299
101	Rational Design of Single Molybdenum Atoms Anchored on N-Doped Carbon for Effective Hydrogen Evolution Reaction. <i>Angewandte Chemie</i> , <b>2017</b> , 129, 16302-16306	3.6	66



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98	Supramolecular Porphyrin Cages Assembled at Molecular-Materials Interfaces for Electrocatalytic CO Reduction. <i>ACS Central Science</i> , <b>2017</b> , 3, 1032-1040	16.8	47
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