

# Sheng-Gang Li

## List of Publications by Citations

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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.

184 papers	6,163 citations	35 h-index	74 g-index
195 ext. papers	7,876 ext. citations	7.1 avg, IF	6.13 L-index

#	Paper	IF	Citations
184	Pillararenes, a new class of macrocycles for supramolecular chemistry. <i>Accounts of Chemical Research</i> , <b>2012</b> , 45, 1294-308	24.3	1081
183	Direct conversion of CO into liquid fuels with high selectivity over a bifunctional catalyst. <i>Nature Chemistry</i> , <b>2017</b> , 9, 1019-1024	17.6	498
182	Insight into methanol synthesis from CO <sub>2</sub> hydrogenation on Cu(1 1 1): Complex reaction network and the effects of H <sub>2</sub> O. <i>Journal of Catalysis</i> , <b>2011</b> , 281, 199-211	7.3	274
181	Direct Production of Lower Olefins from CO <sub>2</sub> Conversion via Bifunctional Catalysis. <i>ACS Catalysis</i> , <b>2018</b> , 8, 571-578	13.1	232
180	Stable High-Index Faceted Pt Skin on Zigzag-Like PtFe Nanowires Enhances Oxygen Reduction Catalysis. <i>Advanced Materials</i> , <b>2018</b> , 30, 1705515	24	223
179	Metal-Free Nitrogen-Doped Mesoporous Carbon for Electroreduction of CO to Ethanol. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 10840-10844	16.4	214
178	Exclusive Formation of Formic Acid from CO Electroreduction by a Tunable Pd-Sn Alloy. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 12219-12223	16.4	196
177	Direct Transformation of Syngas to Aromatics over Na-Zn-Fe 5 C 2 and Hierarchical HZSM-5 Tandem Catalysts. <i>CheM</i> , <b>2017</b> , 3, 323-333	16.2	159
176	The mechanism of potassium promoter: enhancing the stability of active surfaces. <i>Angewandte Chemie - International Edition</i> , <b>2011</b> , 50, 7403-6	16.4	117
175	Relationship between Iron Carbide Phases (Fe <sub>2</sub> C, Fe <sub>7</sub> C <sub>3</sub> , and Fe <sub>5</sub> C <sub>2</sub> ) and Catalytic Performances of Fe/SiO <sub>2</sub> Fischer-Tropsch Catalysts. <i>ACS Catalysis</i> , <b>2018</b> , 8, 3304-3316	13.1	116
174	Effects of Sodium on the Catalytic Performance of CoMn Catalysts for Fischer-Tropsch to Olefin Reactions. <i>ACS Catalysis</i> , <b>2017</b> , 7, 3622-3631	13.1	104
173	Role of zirconium in direct CO <sub>2</sub> hydrogenation to lower olefins on oxide/zeolite bifunctional catalysts. <i>Journal of Catalysis</i> , <b>2018</b> , 364, 382-393	7.3	96
172	Selective Production of Aromatics Directly from Carbon Dioxide Hydrogenation. <i>ACS Catalysis</i> , <b>2019</b> , 9, 3866-3876	13.1	89
171	Rationally designed indium oxide catalysts for CO hydrogenation to methanol with high activity and selectivity. <i>Science Advances</i> , <b>2020</b> , 6, eaaz2060	14.3	84
170	Exploring Furfural Catalytic Conversion on Cu(111) from Computation. <i>ACS Catalysis</i> , <b>2015</b> , 5, 4020-4032	13.1	76
169	Exclusive Formation of Formic Acid from CO <sub>2</sub> Electroreduction by a Tunable Pd-Sn Alloy. <i>Angewandte Chemie</i> , <b>2017</b> , 129, 12387-12391	3.6	72
168	When Density Functional Approximations Meet Iron Oxides. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 5132-5144	6.4	69

167	Understanding of binding energy calibration in XPS of lanthanum oxide by in situ treatment. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 22351-22358	3.6	67
166	Recent advances in the investigation of nanoeffects of Fischer-Tropsch catalysts. <i>Catalysis Today</i> , <b>2018</b> , 311, 8-22	5.3	61
165	Mössbauer Spectroscopy of Iron Carbides: From Prediction to Experimental Confirmation. <i>Scientific Reports</i> , <b>2016</b> , 6, 26184	4.9	58
164	Selective Transformation of CO and H into Lower Olefins over In O -ZnZrO /SAPO-34 Bifunctional Catalysts. <i>ChemSusChem</i> , <b>2019</b> , 12, 3582-3591	8.3	56
163	Helical molecular duplex strands: multiple hydrogen-bond-mediated assembly of self-complementary oligomeric hydrazide derivatives. <i>Journal of Organic Chemistry</i> , <b>2007</b> , 72, 4936-46	4.2	52
162	Novel Heterogeneous Catalysts for CO Hydrogenation to Liquid Fuels. <i>ACS Central Science</i> , <b>2020</b> , 6, 1657-1670	16.7	52
161	Metal-Free Nitrogen-Doped Mesoporous Carbon for Electroreduction of CO <sub>2</sub> to Ethanol. <i>Angewandte Chemie</i> , <b>2017</b> , 129, 10980-10984	3.6	51
160	Molecular Structures, Acid-Base Properties, and Formation of Group 6 Transition Metal Hydroxides. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 8072-8103	3.8	50
159	Direct Production of Higher Oxygenates by Syngas Conversion over a Multifunctional Catalyst. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 4627-4631	16.4	47
158	Mechanism of the Mn Promoter via CoMn Spinel for Morphology Control: Formation of Co <sub>2</sub> C Nanoprisms for Fischer-Tropsch to Olefins Reaction. <i>ACS Catalysis</i> , <b>2017</b> , 7, 8023-8032	13.1	46
157	Mechanisms of Mo <sub>2</sub> C(101)-Catalyzed Furfural Selective Hydrodeoxygenation to 2-Methylfuran from Computation. <i>ACS Catalysis</i> , <b>2016</b> , 6, 6790-6803	13.1	43
156	Fischer-Tropsch Synthesis to Olefins: Catalytic Performance and Structure Evolution of Co <sub>2</sub> C-Based Catalysts under a CO <sub>2</sub> Environment. <i>ACS Catalysis</i> , <b>2019</b> , 9, 9554-9567	13.1	42
155	Cleavage of Covalent Bonds in the Pyrolysis of Lignin, Cellulose, and Hemicellulose. <i>Energy &amp; Fuels</i> , <b>2015</b> , 29, 5773-5780	4.1	42
154	Effects of alkali on iron-based catalysts for Fischer-Tropsch synthesis: CO chemisorptions study. <i>Journal of Molecular Catalysis A</i> , <b>2015</b> , 396, 174-180		41
153	A single-molecule study of the inhibition effect of Naringenin on transforming growth factor- $\alpha$ ligand-receptor binding. <i>Chemical Communications</i> , <b>2011</b> , 47, 5440-2	5.8	41
152	Online Kinetics Study of Oxidative Coupling of Methane over La <sub>2</sub> O <sub>3</sub> for Methane Activation: What Is Behind the Distinguished Light-off Temperatures?. <i>ACS Catalysis</i> , <b>2018</b> , 8, 11761-11772	13.1	37
151	Oxidation, Reduction, and Condensation of Alcohols over (MO <sub>3</sub> ) <sub>3</sub> (M = Mo, W) Nanoclusters. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 22620-22634	3.8	35
150	Noncovalent synthesis of shape-persistent cyclic hexamers from ditopic hydrazide-based supramolecular synthons and asymmetric induction of supramolecular chirality. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 12657-63	16.4	35

149	Correlation between the acid-base properties of the La <sub>2</sub> O <sub>3</sub> catalyst and its methane reactivity. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 16509-17	3.6	32
148	Iron Carbides in Fischer-Tropsch Synthesis: Theoretical and Experimental Understanding in Epsilon-Iron Carbide Phase Assignment. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 21390-21396	3.8	32
147	Morphology control of Co <sub>2</sub> C nanostructures via the reduction process for direct production of lower olefins from syngas. <i>Journal of Catalysis</i> , <b>2018</b> , 366, 289-299	7.3	32
146	Effect of manganese on a potassium-promoted iron-based Fischer-Tropsch synthesis catalyst. <i>Catalysis Letters</i> , <b>2007</b> , 114, 161-168	2.8	31
145	Mutual responsive hydrazide-based low-molecular-mass organic gelators: probing gelation on the molecular level. <i>Chemistry - A European Journal</i> , <b>2008</b> , 14, 5742-6	4.8	31
144	Oxidation mechanism of chalcopyrite revealed by X-ray photoelectron spectroscopy and first principles studies. <i>Applied Surface Science</i> , <b>2018</b> , 427, 233-241	6.7	30
143	Alkalis in iron-based Fischer-Tropsch synthesis catalysts: distribution, migration and promotion. <i>Journal of Chemical Technology and Biotechnology</i> , <b>2017</b> , 92, 1472-1480	3.5	30
142	Enhanced Ethanol Production from CO Electroreduction at Micropores in Nitrogen-Doped Mesoporous Carbon. <i>ChemSusChem</i> , <b>2020</b> , 13, 293-297	8.3	30
141	Enhanced Fischer-Tropsch performances of graphene oxide-supported iron catalysts via argon pretreatment. <i>Catalysis Science and Technology</i> , <b>2018</b> , 8, 1113-1125	5.5	29
140	Morphology control of K <sub>2</sub> O promoter on H <sub>2</sub> g carbide (Fe <sub>5</sub> C <sub>2</sub> ) under Fischer-Tropsch synthesis condition. <i>Catalysis Today</i> , <b>2016</b> , 261, 93-100	5.3	28
139	Controllable deposition of Pt nanoparticles into a KL zeolite by atomic layer deposition for highly efficient reforming of n-heptane to aromatics. <i>Catalysis Science and Technology</i> , <b>2017</b> , 7, 1342-1350	5.5	27
138	Theoretical study on the dissociative adsorption of CH <sub>4</sub> on Pd-doped Ni surfaces. <i>Chinese Journal of Catalysis</i> , <b>2013</b> , 34, 911-922	11.3	26
137	Insights into oil recovery, soil rehabilitation and low temperature behaviors of microwave-assisted petroleum-contaminated soil remediation. <i>Journal of Hazardous Materials</i> , <b>2019</b> , 377, 341-348	12.8	24
136	Efficient production of lactic acid from sugars over Sn-Beta zeolite in water: catalytic performance and mechanistic insights. <i>Sustainable Energy and Fuels</i> , <b>2019</b> , 3, 1163-1171	5.8	24
135	Visible light-driven methanol dehydrogenation and conversion into 1,1-dimethoxymethane over a non-noble metal photocatalyst under acidic conditions. <i>Catalysis Science and Technology</i> , <b>2018</b> , 8, 3372-3378	5.5	24
134	Ultralow Pt Catalyst for Formaldehyde Removal: The Determinant Role of Support. <i>IScience</i> , <b>2018</b> , 9, 487-501	6.1	24
133	In Situ XRD Study on Promotional Effect of Potassium on Carburization of Spray-dried Precipitated Fe <sub>2</sub> O <sub>3</sub> Catalysts. <i>ChemCatChem</i> , <b>2017</b> , 9, 1691-1700	5.2	23
132	Morphology and Reactivity Evolution of HCP and FCC Ru Nanoparticles under CO Atmosphere. <i>ACS Catalysis</i> , <b>2019</b> , 9, 2768-2776	13.1	23

131	Controlled chelation between tannic acid and Fe precursors to obtain N, S co-doped carbon with high density Fe-single atom-nanoclusters for highly efficient oxygen reduction reaction in Zn  air batteries. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 17136-17149	13	23
130	Propagating DFT Uncertainty to Mechanism Determination, Degree of Rate Control, and Coverage Analysis: The Kinetics of Dry Reforming of Methane. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 30389-30397	3.8	23
129	Theoretical study about Mo <sub>2</sub> C(101)-catalyzed hydrodeoxygenation of butyric acid to butane for biomass conversion. <i>Catalysis Science and Technology</i> , <b>2016</b> , 6, 4923-4936	5.5	22
128	Copper Promotion in CO Adsorption and Dissociation on the Fe(100) Surface. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 20472-20480	3.8	22
127	Methane Activations by Lanthanum Oxide Clusters. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 7932-7945	5.8	22
126	Conformational transition behavior around glass transition temperature. <i>Journal of Chemical Physics</i> , <b>2000</b> , 112, 2016-2020	3.9	22
125	Particle Size Effects of Cobalt Carbide for Fischer-Tropsch to Olefins. <i>ACS Catalysis</i> , <b>2019</b> , 9, 798-809	13.1	22
124	Efficient and sustainable transformation of gamma-valerolactone into nylon monomers. <i>Green Chemistry</i> , <b>2016</b> , 18, 691-694	10	21
123	Highly Dispersed Single-Atom Pt and Pt Clusters in the Fe-Modified KL Zeolite with Enhanced Selectivity for n-Heptane Aromatization. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 29858-29867	9.5	21
122	Guest-regulated chirality switching of planar chiral pseudo[1]catenanes. <i>Organic and Biomolecular Chemistry</i> , <b>2018</b> , 16, 2028-2032	3.9	20
121	Highly Efficient and Stable Vanadia-Titania-Sulfate Catalysts for Methanol Oxidation to Methyl Formate: Synthesis and Mechanistic Study. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 6591-6600	3.8	20
120	Highly efficient production of lactic acid from xylose using Sn-beta catalysts. <i>Green Chemistry</i> , <b>2020</b> , 22, 7333-7336	10	20
119	Formic Acid-Induced Controlled-Release Hydrolysis of Microalgae ( <i>Scenedesmus</i> ) to Lactic Acid over Sn-Beta Catalyst. <i>ChemSusChem</i> , <b>2018</b> , 11, 2492-2496	8.3	19
118	A general approach towards efficient catalysis in Pickering emulsions stabilized by amphiphilic RGO-Silica hybrid materials. <i>RSC Advances</i> , <b>2014</b> , 4, 35744-35749	3.7	19
117	Grain Boundary Plays a Key Role in Carbon Diffusion in Carbon Irons Revealed by a ReaxFF Study. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 23191-23199	3.8	19
116	Progress in coal chemical technologies of China. <i>Reviews in Chemical Engineering</i> , <b>2019</b> , 36, 21-66	5	17
115	Catalyst Design for Selective Hydrodeoxygenation of Glycerol to 1,3-Propanediol. <i>ACS Catalysis</i> , <b>2020</b> , 10, 15217-15226	13.1	17
114	Rational Design of Hydrogen-Donor Solvents for Direct Coal Liquefaction. <i>Energy &amp; Fuels</i> , <b>2018</b> , 32, 4715-4723	4.1	17

113	Role of Peroxides on La <sub>2</sub> O <sub>3</sub> Catalysts in Oxidative Coupling of Methane. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 27954-27960	3.8	17
112	ZnZrO <sub>x</sub> integrated with chain-like nanocrystal HZSM-5 as efficient catalysts for aromatics synthesis from CO <sub>2</sub> hydrogenation. <i>Applied Catalysis B: Environmental</i> , <b>2021</b> , 286, 119929	21.8	17
111	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
110	Precursor controlled synthesis of graphene oxide supported iron catalysts for Fischer–Tropsch synthesis. <i>Catalysis Science and Technology</i> , <b>2018</b> , 8, 2883-2893	5.5	16
109	CO <sub>2</sub> Chemisorption and Its Effect on Methane Activation in La <sub>2</sub> O <sub>3</sub> -Catalyzed Oxidative Coupling of Methane. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 2737-2746	3.8	16
108	On the Role of Sn Segregation of Pt–Sn Catalysts for Propane Dehydrogenation. <i>ACS Catalysis</i> , <b>2021</b> , 11, 4401-4410	13.1	16
107	Highly selective production of olefins from syngas with modified ASF distribution model. <i>Applied Catalysis A: General</i> , <b>2018</b> , 563, 146-153	5.1	16
106	Fabrication of different crystallographically oriented TiO <sub>2</sub> nanotube arrays used in dye-sensitized solar cells. <i>RSC Advances</i> , <b>2015</b> , 5, 41120-41124	3.7	15
105	Nanotoroidal tubule assembled from a functionalized oxacalix[4]arene. <i>CrystEngComm</i> , <b>2010</b> , 12, 3502	3.3	15
104	Mechanism of selective and complete oxidation in La <sub>2</sub> O <sub>3</sub> -catalyzed oxidative coupling of methane. <i>Catalysis Science and Technology</i> , <b>2020</b> , 10, 2602-2614	5.5	14
103	First principles investigation of dissociative adsorption of H during CO hydrogenation over cubic and hexagonal InO catalysts. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 3390-3399	3.6	14
102	Self-regeneration of ferrites incorporated into matched matrices for thermochemical CO <sub>2</sub> splitting. <i>Journal of Materials Chemistry A</i> , <b>2016</b> , 4, 5026-5031	13	14
101	First principles studies of CO and O chemisorption on LaO surfaces. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 26799-26811	3.6	14
100	Catalytic Mechanisms of Methanol Oxidation to Methyl Formate on Vanadia–Titania and Vanadia–Titania–Sulfate Catalysts. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 29290-29301	3.8	14
99	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
98	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
97	Gamma-Ray Irradiation to Accelerate Crystallization of Mesoporous Zeolites. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 11325-11329	16.4	13
96	Cu single-atoms embedded in porous carbon nitride for selective oxidation of methane to oxygenates. <i>Chemical Communications</i> , <b>2020</b> , 56, 14677-14680	5.8	13



95	Potassium Tethered Carbons with Unparalleled Adsorption Capacity and Selectivity for Low-Cost Carbon Dioxide Capture from Flue Gas. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2018</b> , 10, 3495-3505	9.5	12
94	Effective control of Ethylene selectivity during Fischer-Tropsch synthesis over polyethylene-glycol enwrapped porous catalyst. <i>Catalysis Communications</i> , <b>2011</b> , 12, 1466-1470	3.2	12
93	The Mechanism of Potassium Promoter: Enhancing the Stability of Active Surfaces. <i>Angewandte Chemie</i> , <b>2011</b> , 123, 7541-7544	3.6	12
92	Investigation of CO oxidation over Au/TiO <sub>2</sub> catalyst through detailed temperature programmed desorption study under low temperature and Operando conditions. <i>Catalysis Today</i> , <b>2018</b> , 307, 84-92	5.3	11
91	Single-Molecule Imaging Reveals the Activation Dynamics of Intracellular Protein Smad3 on Cell Membrane. <i>Scientific Reports</i> , <b>2016</b> , 6, 33469	4.9	11
90	Effect of calcination behaviors on precipitated iron-manganese Fischer-Tropsch synthesis catalyst. <i>Catalysis Letters</i> , <b>2007</b> , 117, 130-135	2.8	11
89	Developing ReaxFF to Visit CO Adsorption and Dissociation on Iron Surfaces. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 27582-27589	3.8	11
88	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
87	Comparative Study of Iron-Based Fischer-Tropsch Synthesis Catalysts Promoted with Strontium or Potassium. <i>Catalysis Letters</i> , <b>2016</b> , 146, 2574-2584	2.8	10
86	Hydrofunctionalization of olefins to value-added chemicals via photocatalytic coupling. <i>Green Chemistry</i> , <b>2018</b> , 20, 3450-3456	10	10
85	Mechanism of Microwave-Assisted Pyrolysis of Glucose to Furfural Revealed by Isotopic Tracer and Quantum Chemical Calculations. <i>ChemSusChem</i> , <b>2017</b> , 10, 3040-3043	8.3	10
84	Synthesis of S-doped AuPbPt alloy nanowire-networks as superior catalysts towards the ORR and HER. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 23906-23918	13	10
83	Tailoring of ammonia reduced graphene oxide into amine functionalized graphene quantum dots through a Hofmann rearrangement. <i>RSC Advances</i> , <b>2016</b> , 6, 34514-34520	3.7	10
82	The role of oxophilic Mo species in Pt/MgO catalysts as extremely active sites for enhanced hydrodeoxygenation of dibenzofuran. <i>Catalysis Science and Technology</i> , <b>2020</b> , 10, 2948-2960	5.5	9
81	CO Direct versus H-Assisted Dissociation on Hydrogen Coadsorbed Fe <sub>5</sub> C <sub>2</sub> Fischer-Tropsch Catalysts. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 20907-20917	3.8	9
80	Preparation, properties, and applications of acrylic-polyurethane hybrid emulsions in extinction electrophoresis. <i>Journal of Applied Polymer Science</i> , <b>2014</b> , 131, n/a-n/a	2.9	9
79	Product Distribution of Fischer-Tropsch Synthesis in Polar Liquids. <i>Chinese Journal of Catalysis</i> , <b>2011</b> , 32, 1790-1802	11.3	9
78	Fischer-Tropsch to olefins over CoMn-based catalysts: Effect of preparation methods. <i>Applied Catalysis A: General</i> , <b>2020</b> , 592, 117414	5.1	9

77	Mechanistic Aspects of CO Activation and C <sub>1</sub> 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
76	Sulfation Roasting of Nickel Oxide-Sulfide Mixed Ore Concentrate in the Presence of Ammonium Sulfate: Experimental and DFT Studies. <i>Metals</i> , <b>2019</b> , 9, 1256	2.3	9
75	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
74	A DFT-based microkinetic study on methanol synthesis from CO hydrogenation over the InO catalyst. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 1888-1895	3.6	9
73	Solvent-Free Synthesis of Mg-Incorporated Nanocrystalline SAPO-34 Zeolites via Natural Clay for Chloromethane-to-Olefin Conversion. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2020</b> , 8, 4185-4193	8.3	8
72	First principles studies on the selectivity of dimethoxymethane and methyl formate in methanol oxidation over VO/TiO-based catalysts. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 19393-19406	3.6	8
71	First principles prediction of CH reactivities with CoO nanocatalysts of different morphologies. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 30874-30882	3.6	8
70	Quantitative Conversion of Methanol to Methyl Formate on Graphene-Confined Nano-Oxides. <i>IScience</i> , <b>2020</b> , 23, 101157	6.1	8
69	Catalytic cycle of the partial oxidation of methane to methanol over Cu-ZSM-5 revealed using DFT calculations. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 4963-4974	3.6	8
68	Valerolactone-introduced controlled-isomerization of glucose for lactic acid production over an Sn-Beta catalyst. <i>Green Chemistry</i> , <b>2021</b> , 23, 2634-2639	10	8
67	Continuous Conversion of Glucose into Methyl Lactate over the Sn-Beta Zeolite: Catalytic Performance and Activity Insight. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2020</b> , 59, 17365-17372	3.9	7
66	Efficient one-pot valorization of ethanol to 1-butanol over an earth-abundant Ni/MgO catalyst under mild conditions. <i>Sustainable Energy and Fuels</i> , <b>2020</b> , 4, 1612-1615	5.8	7
65	Energy dispersive spectrometry and first principles studies on the oxidation of pentlandite. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 12791-12798	3.6	7
64	Electronic Structure and Oxidation Mechanism of Nickel-Copper Converter Matte from First-Principles Calculations. <i>ACS Omega</i> , <b>2020</b> , 5, 20090-20099	3.9	7
63	Effective Macroporous Core-Shell Structure of Alumina-Supported Spinel Ferrite for Carbon Dioxide Splitting Based on Chemical Looping. <i>Energy Technology</i> , <b>2016</b> , 4, 1349-1357	3.5	7
62	Modeling of Gas Solubility in Hydrocarbons Using the Perturbed-Chain Statistical Associating Fluid Theory Equation of State. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2019</b> , 58, 12347-12360	3.9	6
61	Application of the Perturbed-Chain SAFT to Phase Equilibria in the Fischer-Tropsch Synthesis. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2019</b> , 58, 8387-8400	3.9	6
60	Surface structure and morphology evolution of iron borides under dynamic conditions: A theoretical study. <i>Applied Surface Science</i> , <b>2020</b> , 525, 146462	6.7	6



59	Understanding lanthanum oxide surface structure by DFT simulation of oxygen 1s calibrated binding energy in XPS after in situ treatment. <i>Applied Surface Science</i> , <b>2021</b> , 548, 149214	6.7	6
58	Reaction pathways and the role of the carbonates during CO <sub>2</sub> hydrogenation over hexagonal In <sub>2</sub> O <sub>3</sub> catalysts. <i>Applied Surface Science</i> , <b>2021</b> , 542, 148591	6.7	6
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53	H <sub>111</sub> g carbide surfaces induced Pt morphological changes: a theoretical insight. <i>Catalysis Science and Technology</i> , <b>2016</b> , 6, 6726-6738	5.5	5
52	Photocatalytic Coupling of Methanol and Formaldehyde into Ethylene Glycol with High Atomic Efficiency. <i>Catalysis Letters</i> , <b>2018</b> , 148, 2274-2282	2.8	5
51	Depolymerization of poly(trimethylene terephthalate) in supercritical methanol. <i>Journal of Applied Polymer Science</i> , <b>2004</b> , 92, 2363-2368	2.9	5
50	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
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48	CO Self-Promoting Hydrogenation on CO-Saturated Ru(0001): A New Theoretical Insight into How H <sub>2</sub> Participates in CO Activation. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 6508-6515	3.8	4
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46	Formation of radicals in coal pyrolysis examined by electron spin resonance. <i>AIP Advances</i> , <b>2017</b> , 7, 095303	3.5	4
45	Single-molecule fluorescence imaging of membrane-bound proteins for studies of cell signal transduction. <i>Science Bulletin</i> , <b>2011</b> , 56, 1063-1067		4
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43	Theoretical Insights into Morphologies of Alkali-Promoted Cobalt Carbide Catalysts for Fischer-Tropsch Synthesis. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 6061-6072	3.8	4
42	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

41	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
40	Mechanistic studies on millerite chlorination with ammonium chloride. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 4832-4839	3.6	3
39	Mechanistic insights into higher alcohol synthesis from syngas on Rh/Cu single-atom alloy catalysts. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 5070-5077	3.6	3
38	Diesel from Syngas	123-139	3
37	Insights into the High Activity and Methanol Selectivity of the Zn/ZrO <sub>2</sub> Solid Solution Catalyst for CO <sub>2</sub> Hydrogenation. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 27467-27478	3.8	3
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35	Enhanced activity of Mg-Fe-O ferrites for two-step thermochemical CO <sub>2</sub> splitting. <i>Journal of CO<sub>2</sub> Utilization</i> , <b>2018</b> , 26, 544-551	7.6	3
34	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
33	Direct conversion of CO to a jet fuel over CoFe alloy catalysts. <i>Innovation(China)</i> , <b>2021</b> , 2, 100170	17.8	3
32	Bifunctional catalysts with versatile zeolites enable unprecedented para-xylene productivity for syngas conversion under mild conditions. <i>Chem Catalysis</i> , <b>2022</b> ,		3
31	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
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24	Mechanism of oxide-catalyzed selective oxidation: A computational perspective. <i>Annual Reports in Computational Chemistry</i> , <b>2019</b> , 15, 287-333	1.8	2

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21	Conversion of glucose to levulinic acid and upgradation to $\gamma$ -valerolactone on Ru/TiO <sub>2</sub> catalysts. <i>New Journal of Chemistry</i> , <b>2021</b> , 45, 14406-14413	3.6	2
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19	Visualization of on-surface ethylene polymerization through ethylene insertion.. <i>Science</i> , <b>2022</b> , 375, 1188-1191	31.1912	
18	Microwave-induced controlled-isomerization during glucose conversion into lactic acid over a Sn-beta catalyst. <i>Sustainable Energy and Fuels</i> ,	5.8	1
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16	Carburized cobalt catalyst for the Fischer-Tropsch synthesis. <i>Catalysis Science and Technology</i> ,	5.5	1
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4	Efficient one-pot tandem catalysis of glucose into 1,1,2-trimethoxyethane over W-Beta catalysts. <i>Sustainable Energy and Fuels</i> ,	5.8
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