Zhi-Jun Sui

List of Publications by Year
in descending order

59 papers	2,754 citations	201674 27 h-index	182427 51 g-index
59 all docs	59 docs citations	59 times ranked	2377 citing authors

#	Article	IF	Citations
1	First-Principles Calculations of Propane Dehydrogenation over PtSn Catalysts. ACS Catalysis, 2012, 2, 1247-1258.	11.2	235
2	Selective Hydrogenation of Acetylene over Pd-In/Al₂O₃ Catalyst: Promotional Effect of Indium and Composition-Dependent Performance. ACS Catalysis, 2017, 7, 7835-7846.	11.2	194
3	Size-Dependent Reaction Mechanism and Kinetics for Propane Dehydrogenation over Pt Catalysts. ACS Catalysis, 2015, 5, 6310-6319.	11.2	189
4	DFT study of propane dehydrogenation on Pt catalyst: effects of step sites. Physical Chemistry Chemical Physics, 2011, 13, 3257.	2.8	173
5	Density Functional Theory-Assisted Microkinetic Analysis of Methane Dry Reforming on Ni Catalyst. Industrial & Engineering Chemistry Research, 2015, 54, 5901-5913.	3.7	158
6	Size Dependence of Pt Catalysts for Propane Dehydrogenation: from Atomically Dispersed to Nanoparticles. ACS Catalysis, 2020, 10, 12932-12942.	11.2	144
7	Coke Formation on Ptâ€“Sn/Al2O3 Catalyst in Propane Dehydrogenation: Coke Characterization and Kinetic Study. Topics in Catalysis, 2011, 54, 888-896.	2.8	132
8	Dry reforming of methane on Ni-Fe-MgO catalysts: Influence of Fe on carbon-resistant property and kinetics. Applied Catalysis B: Environmental, 2020, 264, 118497.	20.2	122
9	Adsorption Site Regulation to Guide Atomic Design of Niâ€“Ga Catalysts for Acetylene Semiâ€Hydrogenation. Angewandte Chemie - International Edition, 2020, 59, 11647-11652.	13.8	111
10	Coke Formation on Ptâ€“Sn/Al₂O₃ Catalyst for Propane Dehydrogenation. Industrial & Engineering Chemistry Research, 2018, 57, 8647-8654.	3.7	106
11	Reaction mechanism and kinetics for hydrolytic dehydrogenation of ammonia borane on a Pt/CNT catalyst. AIChE Journal, 2017, 63, 60-65.	3.6	90
12	Density functional study of the chemisorption of C1, C2 and C3 intermediates in propane dissociation on Pt(111). Journal of Molecular Catalysis A, 2010, 321, 42-49.	4.8	77
13	Effect of steam addition on the structure and activity of Ptâ€“Sn catalysts in propane dehydrogenation. Chemical Engineering Journal, 2015, 278, 240-248.	12.7	54
14	Tuning selectivity and stability in propane dehydrogenation by shaping Pt particles: A combined experimental and DFT study. Journal of Molecular Catalysis A, 2014, 395, 329-336.	4.8	48
15	High-Throughput Screening of Alloy Catalysts for Dry Methane Reforming. ACS Catalysis, 2021, 11, 8881-8894.	11.2	47
16	Beyond the Reverse Horiutiâ€“Polanyi Mechanism in Propane Dehydrogenation over Pt Catalysts. ACS Catalysis, 2020, 10, 14887-14902.	11.2	44
17	Pore network modeling of catalyst deactivation by coking, from single site to particle, during propane dehydrogenation. AIChE Journal, 2019, 65, 140-150.	3.6	43
18	Improved selectivity and coke resistance of core-shell alloy catalysts for propane dehydrogenation from first principles and microkinetic analysis. Chemical Engineering Journal, 2019, 377, 120049.	12.7	42

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19	Rational Design of Single-Atom-Doped Ga₂O₃ Catalysts for Propane Dehydrogenation: Breaking through Volcano Plot by Lewis Acidâ€“Base Interactions. ACS Catalysis, 2021, 11, 5135-5147.	11.2	41
20	Composition of the Green Oil in Hydrogenation of Acetylene over a Commercial Pdâ€Ag/Al₂O₃ Catalyst. Chemical Engineering and Technology, 2016, 39, 865-873.	1.5	39
21	Tuning Adsorption and Catalytic Properties of Î±-Cr₂O₃ and ZnO in Propane Dehydrogenation by Creating Oxygen Vacancy and Doping Single Pt Atom: A Comparative First-Principles Study. Industrial & Engineering Chemistry Research, 2019, 58, 10199-10209.	3.7	38
22	Structural and Kinetics Understanding of Support Effects in Pd-Catalyzed Semi-Hydrogenation of Acetylene. Engineering, 2021, 7, 103-110.	6.7	36
23	Boosting Sizeâ€Selective Hydrogen Combustion in the Presence of Propene Using Controllable Metal Clusters Encapsulated in Zeolite. Angewandte Chemie - International Edition, 2018, 57, 9770-9774.	13.8	34
24	Kinetics Insights and Active Sites Discrimination of Pd-Catalyzed Selective Hydrogenation of Acetylene. Industrial & Engineering Chemistry Research, 2019, 58, 1888-1895.	3.7	34
25	On the ensemble requirement of fully selective chemical looping methane partial oxidation over La-Fe-based perovskites. Applied Catalysis B: Environmental, 2022, 301, 120788.	20.2	34
26	Adsorption Site Regulation to Guide Atomic Design of Niâ€“Ga Catalysts for Acetylene Semiâ€Hydrogenation. Angewandte Chemie, 2020, 132, 11744-11749.	2.0	31
27	Insights into Hydrogen Transport Behavior on Perovskite Surfaces: Transition from the Grotthuss Mechanism to the Vehicle Mechanism. Langmuir, 2019, 35, 9962-9969.	3.5	29
28	Tailoring catalytic properties of V2O3 to propane dehydrogenation through single-atom doping: A DFT study. Catalysis Today, 2021, 368, 46-57.	4.4	29
29	Hierarchical MgAl2O4 supported Pt-Sn as a highly thermostable catalyst for propane dehydrogenation. Catalysis Communications, 2016, 84, 85-88.	3.3	28
30	Tailoring electronic properties and kinetics behaviors of Pd/Nâ€CNTs catalysts for selective hydrogenation of acetylene. AICHE Journal, 2020, 66, e16857.	3.6	28
31	Dualâ€function catalysis in propane dehydrogenation over <scp>Pt₁â€“Ga₂O₃</scp> catalyst: Insights from a microkinetic analysis. AICHE Journal, 2020, 66, e16232.	3.6	27
32	Support effects of Cs/Al2O3 catalyzed aldol condensation of methyl acetate with formaldehyde. Catalysis Today, 2021, 365, 310-317.	4.4	27
33	Electronic Origin of Oxygen Transport Behavior in La-Based Perovskites: A Density Functional Theory Study. Journal of Physical Chemistry C, 2019, 123, 275-290.	3.1	25
34	Carbon nanofibers supported Ru catalyst for sorbitol hydrogenolysis to glycols: Effect of calcination. Korean Journal of Chemical Engineering, 2010, 27, 1412-1418.	2.7	23
35	Insights into the effects of steam on propane dehydrogenation over a Pt/Al₂O₃ catalyst. Catalysis Science and Technology, 2015, 5, 3991-4000.	4.1	21
36	The role of H₂S addition on Pt/Al₂O₃ catalyzed propane dehydrogenation: a mechanistic study. Catalysis Science and Technology, 2019, 9, 867-876.	4.1	21

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37	Toward rational catalyst design for partial hydrogenation of dimethyl oxalate to methyl glycolate: a descriptor-based microkinetic analysis. Catalysis Science and Technology, 2019, 9, 5763-5773.	4.1	19
38	Structural stability of Lanthanum-based oxygen-deficient perovskites in redox catalysis: A density functional theory study. Catalysis Today, 2020, 347, 142-149.	4.4	18
39	Rational screening of single-atom-doped ZnO catalysts for propane dehydrogenation from microkinetic analysis. Catalysis Science and Technology, 2020, 10, 4938-4951.	4.1	18
40	Hierarchical NiCo LDHâ€“rGO/Ni Foam Composite as Electrode Material for High-Performance Supercapacitors. Transactions of Tianjin University, 2019, 25, 266-275.	6.4	17
41	Selective Oxidation of Hydrogen in the Presence of Propylene over Pt-Based Coreâ€“Shell Nanocatalysts. Journal of Physical Chemistry C, 2015, 119, 21386-21394.	3.1	15
42	Rational design of intermetallic compound catalysts for propane dehydrogenation from a descriptor-based microkinetic analysis. Journal of Catalysis, 2021, 404, 32-45.	6.2	15
43	Effects of Oxygen Vacancy and Pt Doping on the Catalytic Performance of <scp>CeO₂</scp> in Propane Dehydrogenation: A <scp>Firstâ€Principles</scp> Study. Chinese Journal of Chemistry, 2021, 39, 2391-2402.	4.9	13
44	Origin of Chemisorption Energy Scaling Relations over Perovskite Surfaces. Journal of Physical Chemistry C, 2019, 123, 28275-28283.	3.1	11
45	BEEF-vdW+U method applied to perovskites: thermodynamic, structural, electronic, and magnetic properties. Journal of Physics Condensed Matter, 2019, 31, 145901.	1.8	11
46	Identification of Synergistic Actions between Cu⁰ and Cu⁺ Sites in Hydrogenation of Dimethyl Oxalate from Microkinetic Analysis. Industrial & Engineering Chemistry Research, 2020, 59, 22451-22459.	3.7	11
47	Probing the structure sensitivity of dimethyl oxalate partial hydrogenation over Ag nanoparticles: A combined experimental and microkinetic study. Chemical Engineering Science, 2022, 259, 117830.	3.8	9
48	Size-Dependent Segregation Preference in Single-Atom Alloys of Late Transition Metals: Effects of Magnetism, Electron Correlation, and Geometrical Strain. Journal of Physical Chemistry C, 2019, 123, 18417-18424.	3.1	8
49	Surface phase diagrams of La-based perovskites towards the O-rich limit from first principles. Physical Chemistry Chemical Physics, 2019, 21, 12859-12871.	2.8	7
50	Tuning partially charged Pt^{Î´+}of atomically dispersed Pt catalysts toward superior propane dehydrogenation performance. Catalysis Science and Technology, 2021, 11, 7840-7843.	4.1	5
51	Grafting of polystyrene on carbon nanofibers by introducing a methacrylate unit. Polymer International, 2009, 58, 564-569.	3.1	4
52	Boosting Sizeâ€Selective Hydrogen Combustion in the Presence of Propene Using Controllable Metal Clusters Encapsulated in Zeolite. Angewandte Chemie, 2018, 130, 9918-9922.	2.0	4
53	Enhanced catalytic performance of transition metal-doped Cr2O3 catalysts for propane dehydrogenation: A microkinetic modeling study. Chemical Engineering Journal, 2022, 446, 136913.	12.7	4
54	Evaluation of approximations for concentration-dependent micropore diffusion in sorbent with bidisperse pore structure. Adsorption, 2014, 20, 843-853.	3.0	3

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55	A Mechanistic Study of Oxygen Replenishment of Reduced Perovskites in Chemical Looping Redox Reactions. Journal of Physical Chemistry C, 2022, 126, 7431-7445.	3.1	3
56	Catalytic Vapor Decomposition of Methane over Nickle Catalyst: Growth Rate and the Corresponding Microstructures of Carbon Nanofibers. Journal of Chemical Engineering of Japan, 2009, 42, S204-S211.	0.6	2
57	Computer-aided bimetallic catalyst screening for ester selective hydrogenation. Catalysis Science and Technology, 2022, 12, 2761-2765.	4.1	2
58	Thermal stability of nanoparticle supported on Al2O3 with different morphologies. Materials Research Express, 2019, 6, 095064.	1.6	1
59	Effect of hydrogen on the synthesis of carbon nanofibers by CO disproportionation on ultrafine Fe₃O₄. Asia-Pacific Journal of Chemical Engineering, 2009, 4, 590-595.	1.5	0