

Jing Liu

List of Publications by Year in descending order

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160
papers

6,213
citations

44069

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all docs

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docs citations

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times ranked

2904
citing authors

#	ARTICLE	IF	CITATIONS
1	Mechanistic studies of mercury adsorption and oxidation by oxygen over spinel-type MnFe ₂ O ₄ . Journal of Hazardous Materials, 2017, 321, 154-161.	12.4	184
2	Effects of chemical functional groups on elemental mercury adsorption on carbonaceous surfaces. Journal of Hazardous Materials, 2011, 186, 108-113.	12.4	150
3	Reaction mechanism for NH ₃ -SCR of NO _x over CuMn ₂ O ₄ catalyst. Chemical Engineering Journal, 2019, 361, 578-587.	12.7	146
4	Reaction mechanisms and chemical kinetics of mercury transformation during coal combustion. Progress in Energy and Combustion Science, 2020, 79, 100844.	31.2	145
5	Molecular-level insights into mercury removal mechanism by pyrite. Journal of Hazardous Materials, 2018, 344, 104-112.	12.4	138
6	Modeling of homogeneous mercury speciation using detailed chemical kinetics. Combustion and Flame, 2003, 132, 208-218.	5.2	131
7	Effect of SO ₂ on mercury binding on carbonaceous surfaces. Chemical Engineering Journal, 2012, 184, 163-167.	12.7	113
8	Mechanism of Heterogeneous Mercury Oxidation by HBr over V ₂ O ₅ /TiO ₂ Catalyst. Environmental Science & Technology, 2016, 50, 5398-5404.	10.0	109
9	Field Effect Regulation of DNA Translocation through a Nanopore. Analytical Chemistry, 2010, 82, 8217-8225.	6.5	106
10	AMn ₂ O ₄ (A=Cu, Ni and Zn) sorbents coupling high adsorption and regeneration performance for elemental mercury removal from syngas. Journal of Hazardous Materials, 2020, 388, 121738.	12.4	102
11	Density functional study of hydrogen sulfide adsorption mechanism on activated carbon. Fuel Processing Technology, 2018, 171, 258-264.	7.2	98
12	The adsorption mechanism of elemental mercury on CuO (110) surface. Chemical Engineering Journal, 2012, 200-202, 91-96.	12.7	97
13	Theoretical study of mercury species adsorption mechanism on MnO ₂ (110) surface. Chemical Engineering Journal, 2014, 256, 93-100.	12.7	97
14	Insights into the mechanism of heterogeneous mercury oxidation by HCl over V ₂ O ₅ /TiO ₂ catalyst: Periodic density functional theory study. Proceedings of the Combustion Institute, 2015, 35, 2855-2865.	3.9	83
15	Oxidation mechanism of elemental mercury by HCl over MnO ₂ catalyst: Insights from first principles. Chemical Engineering Journal, 2015, 280, 354-362.	12.7	82
16	Experimental and theoretical studies of mercury oxidation over CeO ₂ WO ₃ /TiO ₂ catalysts in coal-fired flue gas. Chemical Engineering Journal, 2017, 317, 758-765.	12.7	82
17	Elemental mercury removal from syngas by porous carbon-supported CuCl ₂ sorbents. Fuel, 2019, 239, 138-144.	6.4	82
18	Insights into the catalytic behavior of LaMnO ₃ perovskite for Hg ₀ oxidation by HCl. Journal of Hazardous Materials, 2020, 383, 121156.	12.4	82

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19	Density functional theory study on the heterogeneous reaction between Hg 0 and HCl over spinel-type MnFe ₂ O ₄ . Chemical Engineering Journal, 2017, 308, 897-903.	12.7	81
20	High CO ₂ adsorption capacities in UiO type MOFs comprising heterocyclic ligand. Microporous and Mesoporous Materials, 2018, 256, 25-31.	4.4	81
21	Heterogeneous reaction mechanism of elemental mercury oxidation by oxygen species over MnO ₂ catalyst. Proceedings of the Combustion Institute, 2019, 37, 2967-2975.	3.9	80
22	Design of O ₂ /SO ₂ dual-doped porous carbon as superior sorbent for elemental mercury removal from flue gas. Journal of Hazardous Materials, 2019, 366, 321-328.	12.4	79
23	FeS ₂ -anchored transition metal single atoms for highly efficient overall water splitting: a DFT computational screening study. Journal of Materials Chemistry A, 2021, 9, 2438-2447.	10.3	73
24	On-Line Analysis and Kinetic Behavior of Arsenic Release during Coal Combustion and Pyrolysis. Environmental Science & Technology, 2015, 49, 13716-13723.	10.0	72
25	Kinetic study of heterogeneous mercury oxidation by HCl on fly ash surface in coal-fired flue gas. Combustion and Flame, 2016, 168, 1-9.	5.2	72
26	Interface reaction activity of recyclable and regenerable Cu-Mn spinel-type sorbent for Hg ₀ capture from flue gas. Chemical Engineering Journal, 2019, 372, 697-707.	12.7	69
27	Heterogeneous Mercury Oxidation by HCl over CeO ₂ Catalyst: Density Functional Theory Study. Journal of Physical Chemistry C, 2015, 119, 15047-15055.	3.1	68
28	Theoretical studies of mercury-bromine species adsorption mechanism on carbonaceous surface. Proceedings of the Combustion Institute, 2013, 34, 2811-2819.	3.9	64
29	Reaction mechanism of CO ₂ methanation over Rh/TiO ₂ catalyst. Fuel, 2020, 276, 118093.	6.4	63
30	Theoretical studies of CO ₂ adsorption mechanism on linkers of metal-organic frameworks. Fuel, 2012, 95, 521-527.	6.4	62
31	Mercury removal by biomass-derived porous carbon: Experimental and theoretical insights into the effect of H ₂ S. Chemical Engineering Journal, 2018, 348, 409-415.	12.7	62
32	Effect of Functionalized Linker on CO ₂ Binding in Zeolitic Imidazolate Frameworks: Density Functional Theory Study. Journal of Physical Chemistry C, 2012, 116, 16985-16991.	3.1	61
33	Effects of Water Vapor and Trace Gas Impurities in Flue Gas on CO ₂ /N ₂ Separation Using ZIF-68. Journal of Physical Chemistry C, 2014, 118, 6744-6751.	3.1	61
34	Construction of an Anion-Pillared MOF Database and the Screening of MOFs Suitable for Xe/Kr Separation. ACS Applied Materials & Interfaces, 2021, 13, 11039-11049.	8.0	60
35	Adsorption and diffusion of carbon dioxide on ZIF-68. Chemical Engineering Science, 2014, 118, 32-40.	3.8	59
36	Reaction mechanism of spinel CuFe ₂ O ₄ with CO during chemical-looping combustion: An experimental and theoretical study. Proceedings of the Combustion Institute, 2019, 37, 4399-4408.	3.9	59

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37	Improving Carbon Dioxide Storage Capacity of Metal Organic Frameworks by Lithium Alkoxide Functionalization: A Molecular Simulation Study. <i>Journal of Physical Chemistry C</i> , 2016, 120, 10311-10319.	3.1	57
38	Heterogeneous reaction kinetics of mercury oxidation by HCl over Fe ₂ O ₃ surface. <i>Fuel Processing Technology</i> , 2017, 159, 266-271.	7.2	57
39	Density functional theory study of mercury adsorption on V ₂ O ₅ (0 0 1) surface with implications for oxidation. <i>Proceedings of the Combustion Institute</i> , 2011, 33, 2771-2777.	3.9	56
40	Theoretical study of stability and reaction mechanism of CuO supported on ZrO ₂ during chemical looping combustion. <i>Applied Surface Science</i> , 2016, 367, 485-492.	6.1	55
41	Theoretical Studies of Properties and Reactions Involving Mercury Species Present in Combustion Flue Gases. <i>Energy & Fuels</i> , 2010, 24, 117-122.	5.1	54
42	Effects of water vapor and trace gas impurities in flue gas on CO ₂ capture in zeolitic imidazolate frameworks: The significant role of functional groups. <i>Fuel</i> , 2017, 200, 244-251.	6.4	54
43	Development of O ₂ and NO Co-Doped Porous Carbon as a High-Capacity Mercury Sorbent. <i>Environmental Science & Technology</i> , 2019, 53, 1725-1731.	10.0	54
44	Mercury oxidation mechanism on Pd(100) surface from first-principles calculations. <i>Chemical Engineering Journal</i> , 2014, 237, 344-351.	12.7	53
45	Quantitative Analysis of Calorific Value of Coal Based on Spectral Preprocessing by Laser-Induced Breakdown Spectroscopy (LIBS). <i>Energy & Fuels</i> , 2018, 32, 24-32.	5.1	52
46	Kinetic mechanism studies on reactions of mercury and oxidizing species in coal combustion. <i>Fuel</i> , 2005, 84, 1215-1220.	6.4	49
47	Charge-distribution modulation of copper ferrite spinel-type catalysts for highly efficient Hg ⁰ oxidation. <i>Journal of Hazardous Materials</i> , 2021, 402, 123576.	12.4	49
48	Experimental study on fly ash capture mercury in flue gas. <i>Science China Technological Sciences</i> , 2010, 53, 976-983.	4.0	48
49	Diffusiophoresis of an Elongated Cylindrical Nanoparticle along the Axis of a Nanopore. <i>ChemPhysChem</i> , 2010, 11, 3281-3290.	2.1	47
50	Performance and mechanism of CuS-modified MWCNTs on mercury removal: Experimental and density functional theory study. <i>Fuel</i> , 2022, 309, 122238.	6.4	47
51	Catalytic reaction mechanism of formaldehyde oxidation by oxygen species over Pt/TiO ₂ catalyst. <i>Chemosphere</i> , 2020, 248, 125980.	8.2	46
52	Mechanistic understanding of CO ₂ hydrogenation to methane over Ni/CeO ₂ catalyst. <i>Applied Surface Science</i> , 2021, 558, 149866.	6.1	46
53	Cost-Effective Manganese Ore Sorbent for Elemental Mercury Removal from Flue Gas. <i>Environmental Science & Technology</i> , 2019, 53, 9957-9965.	10.0	45
54	Ultrasensitive detection of mercury (II) ions using electrochemical surface plasmon resonance with magnetohydrodynamic convection. <i>Journal of Colloid and Interface Science</i> , 2009, 333, 485-490.	9.4	44

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55	Ionic current rectification in a conical nanofluidic field effect transistor. <i>Sensors and Actuators B: Chemical</i> , 2011, 157, 742-751.	7.8	44
56	Effect of the Mechanism of H ₂ S on Elemental Mercury Removal Using the MnO ₂ Sorbent during Coal Gasification. <i>Energy & Fuels</i> , 2018, 32, 4453-4460.	5.1	44
57	Determination of Kinetic Law for Toxic Metals Release during Thermal Treatment of Model Waste in a Fluid-Bed Reactor. <i>Environmental Science & Technology</i> , 2005, 39, 9331-9336.	10.0	43
58	Plasma-Modified N/O-Doped Porous Carbon for CO ₂ Capture: An Experimental and Theoretical Study. <i>Energy & Fuels</i> , 2020, 34, 6077-6084.	5.1	42
59	Study on mechanism of mercury oxidation by fly ash from coal combustion. <i>Science Bulletin</i> , 2010, 55, 163-167.	1.7	40
60	A skeletal reaction scheme for selective catalytic reduction of NO _x with NH ₃ over CeO ₂ /TiO ₂ catalyst. <i>Fuel Processing Technology</i> , 2018, 174, 17-25.	7.2	40
61	Nitrogen/Oxygen Co-Doped Porous Carbon Derived from Biomass for Low-Pressure CO ₂ Capture. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 14055-14063.	3.7	40
62	Kinetic calculation and modeling of trace element reactions during combustion. <i>Powder Technology</i> , 2008, 180, 157-163.	4.2	39
63	Experimental and DFT studies of the role of H ₂ S in Hg ⁰ removal from syngas over CuMn ₂ O ₄ sorbent. <i>Chemical Engineering Journal</i> , 2020, 391, 123616.	12.7	39
64	Comprehensive Hg/Br reaction chemistry over Fe ₂ O ₃ surface during coal combustion. <i>Combustion and Flame</i> , 2018, 196, 210-222.	5.2	37
65	Oxygen-Rich Porous Carbon Derived from Biomass for Mercury Removal: An Experimental and Theoretical Study. <i>Langmuir</i> , 2018, 34, 12049-12057.	3.5	36
66	Water-Soluble Trifunctional Binder for Sulfur Cathodes for Lithium-Sulfur Battery. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 33066-33074.	8.0	36
67	A mechanistic study of CO oxidation over spinel MnFe ₂ O ₄ surface during chemical-looping combustion. <i>Fuel</i> , 2018, 230, 410-417.	6.4	35
68	Mechanism of mercury-iodine species binding on carbonaceous surface: Insight from density functional theory study. <i>Chemical Engineering Journal</i> , 2016, 306, 704-708.	12.7	32
69	Temporal measurements and kinetics of selenium release during coal combustion and gasification in a fluidized bed. <i>Journal of Hazardous Materials</i> , 2016, 310, 40-47.	12.4	32
70	Homogeneous and heterogeneous reaction mechanisms and kinetics of mercury oxidation in coal-fired flue gas with bromine addition. <i>Proceedings of the Combustion Institute</i> , 2017, 36, 4039-4049.	3.9	32
71	Two-dimensional pyrite supported transition metal for highly-efficient electrochemical CO ₂ reduction: A theoretical screening study. <i>Chemical Engineering Journal</i> , 2021, 424, 130541.	12.7	31
72	Understanding A-site tuning effect on formaldehyde catalytic oxidation over La-Mn perovskite catalysts. <i>Journal of Hazardous Materials</i> , 2022, 422, 126931.	12.4	31

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73	Polarization Effect of a Dielectric Membrane on the Ionic Current Rectification in a Conical Nanopore. <i>Journal of Physical Chemistry C</i> , 2011, 115, 24951-24959.	3.1	29
74	Effects of incorporated oxygen and sulfur heteroatoms into ligands for CO ₂ /N ₂ and CO ₂ /CH ₄ separation in metal-organic frameworks: A molecular simulation study. <i>Fuel</i> , 2018, 226, 591-597.	6.4	29
75	Theoretical investigation of sodium capture mechanism on kaolinite surfaces. <i>Fuel</i> , 2018, 234, 318-325.	6.4	29
76	The role of SO ₂ in arsenic removal by carbon-based sorbents: A DFT study. <i>Chemical Engineering Journal</i> , 2021, 410, 128439.	12.7	29
77	Regenerable Co _x Mn _{3-2x} O ₄ spinel sorbents for elemental mercury removal from syngas: Experimental and DFT studies. <i>Fuel</i> , 2020, 266, 117105.	6.4	28
78	On-line measurement and kinetic studies of sodium release during biomass gasification and pyrolysis. <i>Fuel</i> , 2016, 178, 202-208.	6.4	27
79	Density Functional Theory Study on the Reaction Mechanism of Spinel CoFe ₂ O ₄ with CO during Chemical-Looping Combustion. <i>Journal of Physical Chemistry C</i> , 2019, 123, 17335-17342.	3.1	27
80	Strong binding site molarity of MOFs and its effect on CO ₂ adsorption. <i>Microporous and Mesoporous Materials</i> , 2015, 214, 242-245.	4.4	26
81	O ₂ and CO ₂ Mixed Gas Production Using a Zr-Doped Cu-Based Oxygen Carrier. <i>Industrial & Engineering Chemistry Research</i> , 2015, 54, 9805-9812.	3.7	26
82	Effects of functional groups for CO ₂ capture using metal organic frameworks. <i>Frontiers of Chemical Science and Engineering</i> , 2021, 15, 437-449.	4.4	26
83	A catalytic reaction scheme for NO reduction by CO over Mn-terminated LaMnO ₃ perovskite: A DFT study. <i>Fuel Processing Technology</i> , 2021, 216, 106798.	7.2	26
84	Electrochemical conversion of CO ₂ to syngas over Cu-M (M = Cd, Zn, Ni, Ag, and Pd) bimetal catalysts. <i>Fuel</i> , 2021, 304, 121341.	6.4	26
85	Experimental and theoretical studies of cadmium adsorption over Fe ₂ O ₃ sorbent in incineration flue gas. <i>Chemical Engineering Journal</i> , 2021, 425, 131647.	12.7	26
86	Mechanism of CO ₂ adsorption on Mg/DOBDC with elevated CO ₂ loading. <i>Fuel</i> , 2016, 181, 340-346.	6.4	25
87	Insights into the mechanism of lead species adsorption over Al ₂ O ₃ sorbent. <i>Journal of Hazardous Materials</i> , 2021, 413, 125371.	12.4	25
88	Bimetallic Fe-Cu-Based Metal-Organic Frameworks as Efficient Adsorbents for Gaseous Elemental Mercury Removal. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 781-789.	3.7	25
89	Theoretical prediction the removal of mercury from flue gas by MOFs. <i>Fuel</i> , 2016, 184, 474-480.	6.4	24
90	Comprehensive evolution mechanism of SO _x formation during pyrite oxidation. <i>Proceedings of the Combustion Institute</i> , 2019, 37, 2809-2819.	3.9	24

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91	Molecular Mechanistic Nature of Elemental Mercury Oxidation by Surface Oxygens over the Co_3O_4 Catalyst. <i>Journal of Physical Chemistry C</i> , 2020, 124, 4605-4612.	3.1	24
92	Efficient capture of gaseous elemental mercury based on novel copper-based metal-organic frameworks. <i>Fuel</i> , 2021, 289, 119791.	6.4	24
93	Molecular study of heterogeneous mercury conversion mechanism over Cu-MOFs: Oxidation pathway and effect of halogen. <i>Fuel</i> , 2021, 290, 120030.	6.4	24
94	Studies on the synergistically improved reactivity of spinel NiFe_2O_4 oxygen carrier for chemical-looping combustion. <i>Energy</i> , 2022, 239, 122100.	8.8	24
95	Highly Selective Separations of $\text{C}_2\text{H}_2/\text{C}_2\text{H}_4$ and $\text{C}_2\text{H}_2/\text{C}_2\text{H}_6$ in Metal-Organic Frameworks via Pore Environment Design. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 19946-19957.	3.7	22
96	Elucidating the mechanism of Hg_0 oxidation by chlorine species over Co_3O_4 catalyst at molecular level. <i>Applied Surface Science</i> , 2020, 513, 145885.	6.1	22
97	Experimental and Theoretical Insights into the Effect of Syngas Components on Hg_0 Removal over CoMn_2O_4 Sorbent. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 8078-8085.	3.7	22
98	Roles of Oxygen Functional Groups in Hydrogen Sulfide Adsorption on Activated Carbon Surface: A Density Functional Study. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 5526-5532.	3.7	20
99	Mercury/oxygen reaction mechanism over CuFe_2O_4 catalyst. <i>Journal of Hazardous Materials</i> , 2022, 424, 127556.	12.4	20
100	Temporal influence of reaction atmosphere and chlorine on arsenic release in combustion, gasification and pyrolysis of sawdust. <i>Journal of Hazardous Materials</i> , 2020, 382, 121047.	12.4	19
101	Nickel Nanoparticles Encapsulated in SSZ-13 Cage for Highly Efficient CO_2 Hydrogenation. <i>Energy & Fuels</i> , 2021, 35, 13240-13248.	5.1	19
102	Crystal orientation effects on the electrochemical conversion of CO_2 to syngas over Cu-M ($\text{M}=\text{Ag, Ni}$). <i>Journal of Electroanalytical Chemistry</i> , 2021, 898, 140000.	6.1	19
103	Insights into the effect of chlorine on arsenic release during MSW incineration: An on-line analysis and kinetic study. <i>Waste Management</i> , 2018, 75, 327-332.	7.4	18
104	Enhanced photocatalytic Hg_0 oxidation activity of iodine doped bismuth molybdate (Bi_2MoO_6) under visible light. <i>Journal of Colloid and Interface Science</i> , 2022, 607, 1864-1875.	9.4	18
105	Experimental and theoretical study of arsenic removal by porous carbon from MSW incineration flue gas. <i>Fuel</i> , 2022, 312, 123000.	6.4	18
106	Insights into the Effects of Atmosphere and Chlorine on Potassium Release during Biomass Combustion: Temporal Measurement and Kinetic Studies. <i>Energy & Fuels</i> , 2018, 32, 12523-12531.	5.1	17
107	Metal-Organic Frameworks Grafted by Univariate and Multivariate Heterocycles for Enhancing CO_2 Capture: A Molecular Simulation Study. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 2195-2205.	3.7	17
108	A complete catalytic reaction scheme for Hg_0 oxidation by HCl over $\text{RuO}_2/\text{TiO}_2$ catalyst. <i>Journal of Hazardous Materials</i> , 2019, 373, 660-670.	12.4	17

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109	Mechanistic investigation of elemental mercury adsorption over silver-modified vanadium silicate: A DFT study. <i>Journal of Hazardous Materials</i> , 2021, 404, 124108.	12.4	17
110	Reaction mechanism of elemental mercury oxidation to HgSO ₄ during SO ₂ /SO ₃ conversion over V ₂ O ₅ /TiO ₂ catalyst. <i>Proceedings of the Combustion Institute</i> , 2021, 38, 4317-4325.	3.9	17
111	Experimental and theoretical insights into the reaction mechanism of spinel CuMn ₂ O ₄ with CO in chemical-looping combustion. <i>Applied Surface Science</i> , 2021, 561, 150065.	6.1	17
112	High-Throughput Screening of Anion-Pillared Metal-Organic Frameworks for the Separation of Light Hydrocarbons. <i>Journal of Physical Chemistry C</i> , 2021, 125, 20076-20086.	3.1	17
113	Nanosized Zn-In Spinel-Type Sorbents for Elemental Mercury Removal from Flue Gas. <i>Energy & Fuels</i> , 2020, 34, 12853-12859.	5.1	16
114	Temporal release behavior of potassium during pyrolysis and gasification of sawdust particles. <i>Renewable Energy</i> , 2020, 156, 98-106.	8.9	16
115	Experimental and theoretical studies on formaldehyde catalytic combustion over Cu-Fe spinel-type catalyst. <i>Proceedings of the Combustion Institute</i> , 2021, 38, 6483-6491.	3.9	16
116	Mechanistic insights into benzene oxidation over CuMn ₂ O ₄ catalyst. <i>Journal of Hazardous Materials</i> , 2022, 431, 128640.	12.4	16
117	Rational design via surface engineering on dual 2-dimensional ZnSe/g-C ₃ N ₄ heterojunction for efficient sequestration of elemental mercury. <i>Chemical Engineering Journal</i> , 2022, 448, 137606.	12.7	16
118	Molecular-Level Insights into Effect Mechanism of H ₂ S on Mercury Removal by Activated Carbon. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 7889-7897.	3.7	15
119	Computational Screening of Alkali, Alkaline Earth, and Transition Metals Alkoxide-Functionalized Metal-Organic Frameworks for CO ₂ Capture. <i>Journal of Physical Chemistry C</i> , 2018, 122, 19015-19024.	3.1	15
120	Nature of Active Sites and an Oxygen-Assisted Reaction Mechanism for Mercury Capture by Spinel-Type CuMn ₂ O ₄ Sorbents. <i>Energy & Fuels</i> , 2019, 33, 8920-8926.	5.1	15
121	Theoretical Investigation of Arsenic and Selenium Species Adsorption Behavior on Different Mineral Adsorbents. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 23559-23566.	3.7	15
122	As ₂ O ₃ capture from incineration flue gas by Fe ₂ O ₃ -modified porous carbon: Experimental and DFT insights. <i>Fuel</i> , 2022, 321, 124079.	6.4	15
123	Release of Na from sawdust during air and oxy-fuel combustion: A combined temporal detection, thermodynamics and kinetic study. <i>Fuel</i> , 2018, 221, 249-256.	6.4	14
124	Experimental and theoretical insights into the mechanism of spinel CoFe ₂ O ₄ reduction in CO chemical looping combustion. <i>Fuel</i> , 2021, 293, 120473.	6.4	14
125	Mechanistic study of the effect of oxygen vacancy and sulfur poisoning on the reaction of copper ferrite spinel with CO during chemical-looping combustion. <i>Fuel</i> , 2021, 299, 120931.	6.4	14
126	Nanosized Cu-In spinel-type sulfides as efficient sorbents for elemental mercury removal from flue gas. <i>Science of the Total Environment</i> , 2021, 796, 149094.	8.0	14

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127	Two-dimensional WS ₂ as a new mercury removal material: Mercury conversion pathway and effect of defect. <i>Fuel</i> , 2022, 307, 121864.	6.4	14
128	Metal–Metal Interactions of Ternary Spinel for Efficient NH ₃ Selective Catalytic Reduction of NO _x at a Low Temperature. <i>Energy & Fuels</i> , 2020, 34, 15424-15432.	5.1	13
129	Electrocatalytic reduction of CO ₂ to C ₁ products over bimetal catalysts: A DFT screening study. <i>Fuel Processing Technology</i> , 2022, 233, 107315.	7.2	13
130	Theoretical study of reduction mechanism of Fe ₂ O ₃ by H ₂ during chemical looping combustion. <i>Chinese Journal of Chemical Engineering</i> , 2021, 37, 175-183.	3.5	12
131	Review on the Theoretical Understanding of Oxygen Carrier Development for Chemical-Looping Technologies. <i>Energy & Fuels</i> , 2022, 36, 9373-9384.	5.1	12
132	Ab Initio Study of Gas Adsorption in Metal–Organic Frameworks Modified by Lithium: The Significant Role of Li-Containing Functional Groups. <i>Journal of Physical Chemistry C</i> , 2018, 122, 18395-18404.	3.1	11
133	Exploring reaction mechanism of CO oxidation over SrCoO ₃ catalyst: A DFT study. <i>Applied Surface Science</i> , 2021, 570, 151234.	6.1	11
134	Kinetics of heavy metal vaporization from coal in a fluidized bed by an inverse model. <i>Asia-Pacific Journal of Chemical Engineering</i> , 2010, 5, 266-273.	1.5	10
135	Metal-organic frameworks chelated by zinc fluorides for ultra-high affinity to acetylene during C ₂ /C ₁ separations. <i>Fuel</i> , 2020, 266, 117037.	6.4	10
136	Theoretical insights into H ₂ S reaction mechanism over CuFe ₂ O ₄ oxygen carrier. <i>Journal of the Energy Institute</i> , 2021, 99, 120-126.	5.3	10
137	Tunable Cu–M bimetal catalysts enable syngas electrosynthesis from carbon dioxide. <i>New Journal of Chemistry</i> , 2022, 46, 1203-1209.	2.8	9
138	Effect mechanism of NO on electrocatalytic reduction of CO ₂ to CO over Pd@Cu bimetal catalysts. <i>Fuel</i> , 2022, 323, 124339.	6.4	9
139	Chelation of transition metals into MOFs as a promising method for enhancing CO ₂ capture: A computational study. <i>AIChE Journal</i> , 2020, 66, e16835.	3.6	8
140	CO ₂ -mediated sulfur evolution chemistry of pyrite oxidation during oxy-fuel combustion. <i>Combustion and Flame</i> , 2020, 218, 75-83.	5.2	8
141	Reaction mechanism of dichloromethane oxidation on LaMnO ₃ perovskite. <i>Chemosphere</i> , 2021, 277, 130194.	8.2	8
142	Vacancy-mediated transition metals as efficient electrocatalysts for water splitting. <i>Nanoscale</i> , 2022, 14, 7181-7188.	5.6	8
143	Mechanistic Landscape of HCl-Mediated Hg ⁰ Capture by Magnetite. <i>Journal of Physical Chemistry C</i> , 2019, 123, 30434-30442.	3.1	7
144	Molecular Understanding of Heterogeneous Mercury Adsorption and Oxidation Mechanisms over the CuCl ₂ /TiO ₂ Sorbent. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 12610-12616.	3.7	7

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145	Different Reactivities of the (100) and (110) Surfaces of the NiFe ₂ O ₄ Composite Oxygen Carrier in Chemical Looping Combustion: An Atomic Insight. <i>Journal of Physical Chemistry C</i> , 2021, 125, 19190-19199.	3.1	7
146	Computational Design of Porous Framework Materials with Transition-Metal Alkoxide Ligands for Highly Selective Separation of N ₂ over CH ₄ . <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 378-386.	3.7	7
147	Porous aromatic frameworks with metallized catecholate ligands for CO ₂ capture from gas mixtures: A molecular simulation study. <i>Fuel</i> , 2022, 319, 123768.	6.4	7
148	Computational screening of heterocycle decorations in metal-organic frameworks for efficient C ₂ /C ₁ adsorption and separation. <i>Fuel</i> , 2020, 279, 118431.	6.4	6
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