

Yu Zhang

List of Publications by Year in descending order

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759233

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times ranked

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citing authors

#	ARTICLE	IF	CITATIONS
1	Removal and transformation mechanisms of nitrogen and sulfur in petcoke supercritical water gasification via ReaxFF simulation. <i>Molecular Simulation</i> , 2022, 48, 209-220.	2.0	6
2	Investigation of Competitive Adsorption Properties of CO/CO ₂ /O ₂ onto the Kailuan Coals by Molecular Simulation. <i>ACS Omega</i> , 2022, 7, 19305-19318.	3.5	5
3	A large-scale molecular model of Fenghuangshan anthracite coal. <i>Fuel</i> , 2021, 295, 120616.	6.4	29
4	Investigation of the Adsorption Behavior of Organic Sulfur in Coal via Density Functional Theory (DFT) Calculation and Molecular Simulation. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7358-7368.	2.5	2
5	Molecular Simulation of the Adsorption Behaviors of CO ₂ /CH ₄ in Curvature, Planar, and Mixture Models. <i>Energy & Fuels</i> , 2020, 34, 4153-4161.	5.1	12
6	ReaxFF MD simulations of petroleum coke CO ₂ gasification examining the S/N removal mechanisms and CO/CO ₂ reactivity. <i>Fuel</i> , 2019, 257, 116051.	6.4	17
7	Reductive Gaseous (H ₂ /NH ₃) Desulfurization and Gasification of High-Sulfur Petroleum Coke via Reactive Force Field Molecular Dynamics Simulations. <i>Energy & Fuels</i> , 2019, 33, 8065-8075.	5.1	14
8	Structural Differences of Spontaneous Combustion Prone Inertinite-Rich Chinese Lignite Coals: Insights from XRD, Solid-State ¹³ C NMR, LDIMS, and HRTEM. <i>Energy & Fuels</i> , 2019, 33, 4575-4584.	5.1	29
9	Structural features of Qingdao petroleum coke from HRTEM lattice fringes: Distributions of length, orientation, stacking, curvature, and a large-scale image-guided 3D atomistic representation. <i>Carbon</i> , 2018, 129, 790-802.	10.3	91
10	Sulfur removal from petroleum coke during high-temperature pyrolysis. Analysis from TG-MS data and ReaxFF simulations. <i>Journal of Analytical and Applied Pyrolysis</i> , 2018, 132, 134-142.	5.5	51
11	Impact of the crystallite parameters and coal ranks on oxidation and combustion properties of Carboniferous coals and Jurassic coals. <i>Arabian Journal of Geosciences</i> , 2018, 11, 1.	1.3	7
12	ReaxFF simulations of petroleum coke sulfur removal mechanisms during pyrolysis and combustion. <i>Combustion and Flame</i> , 2018, 198, 146-157.	5.2	54
13	Thiophenic Sulfur Transformation in a Carbon Anode during the Aluminum Electrolysis Process. <i>Energy & Fuels</i> , 2017, 31, 4539-4547.	5.1	19
14	Reduction and Desulfurization of Petroleum Coke in Ammonia and Their Thermodynamics. <i>Energy & Fuels</i> , 2016, 30, 3385-3391.	5.1	28
15	Effect of high-temperature pyrolysis on the structure and properties of coal and petroleum coke. <i>Journal of Analytical and Applied Pyrolysis</i> , 2016, 117, 64-71.	5.5	42
16	Mutual Inhibition between Catalytic Impurities of Sulfur and Those of Calcium in Coke during Carbon-Air and Carbon-CO ₂ Reactions. <i>Energy & Fuels</i> , 2015, 29, 1961-1971.	5.1	11
17	Modeling the Change of Green Coke to Calcined Coke Using Qingdao High-Sulfur Petroleum Coke. <i>Energy & Fuels</i> , 2015, 29, 3345-3352.	5.1	44