Jennifer Wilcox

List of Publications by Year
in descending order

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88 papers	9,276 citations	57631 44 h-index	60497 81 g-index
90 all docs	90 docs citations	90 times ranked	10341 citing authors

#	Article	IF	Citations
1	Carbon capture and storage (CCS): the way forward. Energy and Environmental Science, 2018, 11, 1062-1176.	15.6	2,378
2	Negative emissionsâ€”Part 1: Research landscape and synthesis. Environmental Research Letters, 2018, 13, 063001.	2.2	498
3	Hierarchical N-Doped Carbon as CO₂ Adsorbent with High CO₂ Selectivity from Rationally Designed Polypyrrole Precursor. Journal of the American Chemical Society, 2016, 138, 1001-1009.	6.6	405
4	Economic and energetic analysis of capturing CO ₂ from ambient air. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 20428-20433.	3.3	388
5	Advances on methane steam reforming to produce hydrogen through membrane reactors technology: A review. Catalysis Reviews - Science and Engineering, 2016, 58, 1-35.	5.7	261
6	Mercury adsorption and oxidation in coal combustion and gasification processes. International Journal of Coal Geology, 2012, 90-91, 4-20.	1.9	251
7	CO 2 capture from the industry sector. Progress in Energy and Combustion Science, 2017, 63, 146-172.	15.8	247
8	Effects of Surface Heterogeneity on the Adsorption of CO₂ in Microporous Carbons. Environmental Science & Technology, 2012, 46, 1940-1947.	4.6	243
9	A review of direct air capture (DAC): scaling up commercial technologies and innovating for the future. Progress in Energy, 2021, 3, 032001.	4.6	220
10	Ultrahigh Surface Area Three-Dimensional Porous Graphitic Carbon from Conjugated Polymeric Molecular Framework. ACS Central Science, 2015, 1, 68-76.	5.3	207
11	DFT-Based Study on Oxygen Adsorption on Defective Graphene-Supported Pt Nanoparticles. Journal of Physical Chemistry C, 2011, 115, 22742-22747.	1.5	200
12	Molecular Simulation Studies of CO₂ Adsorption by Carbon Model Compounds for Carbon Capture and Sequestration Applications. Environmental Science & Technology, 2013, 47, 95-101.	4.6	192
13	DFT Studies on the Interaction of Defective Graphene-Supported Fe and Al Nanoparticles. Journal of Physical Chemistry C, 2011, 115, 8961-8970.	1.5	175
14	CO₂Adsorption on Carbon Models of Organic Constituents of Gas Shale and Coal. Environmental Science & Technology, 2011, 45, 809-814.	4.6	163
15	Molecular simulation of CO2 adsorption in micro- and mesoporous carbons with surface heterogeneity. International Journal of Coal Geology, 2012, 104, 83-95.	1.9	156
16	Carbon Capture. , 2012, , .		144
17	Methane and CO₂ Adsorption Capacities of Kerogen in the Eagle Ford Shale from Molecular Simulation. Accounts of Chemical Research, 2017, 50, 1818-1828.	7.6	130
18	Tunable Polyanilineâ€Based Porous Carbon with Ultrahigh Surface Area for CO₂ Capture at Elevated Pressure. Advanced Energy Materials, 2016, 6, 1502491.	10.2	129

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19	Molecular simulation and experimental characterization of the nanoporous structures of coal and gas shale. International Journal of Coal Geology, 2014, 121, 123-128.	1.9	128
20	Klinkenberg effect on predicting and measuring helium permeability in gas shales. International Journal of Coal Geology, 2014, 123, 62-68.	1.9	125
21	Role of WO₃ in the Hg Oxidation across the V₂O₅â€“WO₃â€“TiO₂ SCR Catalyst: A DFT Study. Journal of Physical Chemistry C, 2013, 117, 24397-24406.	1.5	107
22	Heterogeneous Mercury Oxidation on Au(111) from First Principles. Environmental Science & Technology, 2013, 47, 8515-8522.	4.6	103
23	Mercury binding on activated carbon. Environmental Progress, 2006, 25, 319-326.	0.8	101
24	Ambient weathering of magnesium oxide for CO2 removal from air. Nature Communications, 2020, 11, 3299.	5.8	95
25	Carbon Capture and Utilization in the Industrial Sector. Environmental Science & Technology, 2017, 51, 11440-11449.	4.6	91
26	Solubility of Hydrogen in PdAg and PdAu Binary Alloys Using Density Functional Theory. Journal of Physical Chemistry B, 2006, 110, 24549-24558.	1.2	87
27	Heterogeneous Mercury Reaction Chemistry on Activated Carbon. Journal of the Air and Waste Management Association, 2011, 61, 418-426.	0.9	80
28	Cost Analysis of Direct Air Capture and Sequestration Coupled to Low-Carbon Thermal Energy in the United States. Environmental Science & Technology, 2020, 54, 7542-7551.	4.6	80
29	Molecular modeling of carbon dioxide transport and storage in porous carbon-based materials. Microporous and Mesoporous Materials, 2012, 158, 195-203.	2.2	79
30	Advancing Adsorption and Membrane Separation Processes for the Gigaton Carbon Capture Challenge. Annual Review of Chemical and Biomolecular Engineering, 2014, 5, 479-505.	3.3	79
31	Observations and Assessment of Fly Ashes from High-Sulfur Bituminous Coals and Blends of High-Sulfur Bituminous and Subbituminous Coals: Environmental Processes Recorded at the Macro- and Nanometer Scale. Energy & Fuels, 2015, 29, 7168-7177.	2.5	79
32	Mercury Species and SO₂ Adsorption on CaO(100). Journal of Physical Chemistry C, 2008, 112, 16484-16490.	1.5	73
33	Natural gas steam reforming reaction at low temperature and pressure conditions for hydrogen production via Pd/PSS membrane reactor. Journal of Membrane Science, 2017, 522, 343-350.	4.1	68
34	High-performance oxygen reduction and evolution carbon catalysis: From mechanistic studies to device integration. Nano Research, 2017, 10, 1163-1177.	5.8	66
35	Cost Analysis of Carbon Capture and Sequestration of Process Emissions from the U.S. Industrial Sector. Environmental Science & Technology, 2020, 54, 7524-7532.	4.6	66
36	Utilization of mineral carbonation products: current state and potential. , 2019, 9, 1096-1113.		65

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37	Impact of alkalinity sources on the life-cycle energy efficiency of mineral carbonation technologies. Energy and Environmental Science, 2012, 5, 8631.	15.6	64
38	Hydrogen production via natural gas steam reforming in a Pd-Au membrane reactor. Comparison between methane and natural gas steam reforming reactions. Journal of Membrane Science, 2018, 568, 113-120.	4.1	64
39	Slippage and viscosity predictions in carbon micropores and their influence on CO2 and CH4 transport. Journal of Chemical Physics, 2013, 138, 064705.	1.2	62
40	First-Principles Investigation of Mercury Adsorption on the Î±-Fe₂O₃(11Ì…02) Surface. Journal of Physical Chemistry C, 2015, 119, 26512-26518.	1.5	60
41	Selection of Shale Preparation Protocol and Outgas Procedures for Applications in Low-Pressure Analysis. Energy & Fuels, 2017, 31, 9043-9051.	2.5	60
42	A Density Functional Theory Study of the Charge State of Hydrogen in Metal Hydrides. Journal of Physical Chemistry C, 2010, 114, 10978-10985.	1.5	53
43	Investigation of Adsorption Behavior of Mercury on Au(111) from First Principles. Environmental Science & Technology, 2012, 46, 7260-7266.	4.6	51
44	A Kinetic Investigation of High-Temperature Mercury Oxidation by Chlorine. Journal of Physical Chemistry A, 2009, 113, 6633-6639.	1.1	50
45	Hg Binding on Pd Binary Alloys and Overlays. Journal of Physical Chemistry C, 2009, 113, 7813-7820.	1.5	49
46	Methylene Blue Adsorption on the Basal Surfaces of Kaolinite: Structure and Thermodynamics from Quantum and Classical Molecular Simulation. Clays and Clay Minerals, 2015, 63, 185-198.	0.6	45
47	Cost Analysis of Carbon Capture and Sequestration from U.S. Natural Gas-Fired Power Plants. Environmental Science & Technology, 2020, 54, 6272-6280.	4.6	44
48	Nitrogen Adsorption, Dissociation, and Subsurface Diffusion on the Vanadium (110) Surface: A DFT Study for the Nitrogen-Selective Catalytic Membrane Application. Journal of Physical Chemistry C, 2014, 118, 4238-4249.	1.5	39
49	CO₂ Storage and Flow Capacity Measurements on Idealized Shales from Dynamic Breakthrough Experiments. Energy & Fuels, 2017, 31, 1193-1207.	2.5	38
50	Mercury Interaction with the Fine Fraction of Coal-Combustion Fly Ash in a Simulated Coal Power Plant Flue Gas Stream. Energy & Fuels, 2015, 29, 6025-6038.	2.5	37
51	Natural Gas vs. Electricity for Solvent-Based Direct Air Capture. Frontiers in Climate, 2021, 2, .	1.3	35
52	Environmental trade-offs of direct air capture technologies in climate change mitigation toward 2100. Nature Communications, 2022, 13, .	5.8	35
53	Revisiting film theory to consider approaches for enhanced solvent-process design for carbon capture. Energy and Environmental Science, 2014, 7, 1769.	15.6	34
54	Consideration of a nitrogen-selective membrane for postcombustion carbon capture through process modeling and optimization. Journal of Membrane Science, 2014, 465, 177-184.	4.1	32

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55	Understanding Deviations in Hydrogen Solubility Predictions in Transition Metals through First-Principles Calculations. Journal of Physical Chemistry C, 2015, 119, 19642-19653.	1.5	31
56	Current state of industrial heating and opportunities for decarbonization. Progress in Energy and Combustion Science, 2022, 91, 100982.	15.8	31
57	Ab initio-based Mercury Oxidation Kinetics via Bromine at Postcombustion Flue Gas Conditions. Energy & Fuels, 2011, 25, 1348-1356.	2.5	30
58	Surface reactivity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">V</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>5</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>(001): Effects	1.1	29
59	Supported Pd-Au Membrane Reactor for Hydrogen Production: Membrane Preparation, Characterization and Testing. Molecules, 2016, 21, 581.	1.7	29
60	Density functional theory investigation of the interaction of water with<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î±</mml:mi><mml:mo>â^'</mml:mo><mml:msub><mml:mi mathvariant="normal">Al</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î±</mml:mi></m. Physic	1.1	26
61	Idealized Shale Sorption Isotherm Measurements To Determine Pore Capacity, Pore Size Distribution, and Surface Area. Energy & Fuels, 2019, 33, 665-676.	2.5	22
62	Molecular simulations of nitrogen-doped hierarchical carbon adsorbents for post-combustion CO₂ capture. Physical Chemistry Chemical Physics, 2016, 18, 28747-28758.	1.3	21
63	Performance of Pd-Based Membranes and Effects of Various Gas Mixtures on H2 Permeation. Environments - MDPI, 2018, 5, 128.	1.5	21
64	Design and operations optimization of membrane-based flexible carbon capture. International Journal of Greenhouse Gas Control, 2019, 84, 154-163.	2.3	21
65	Direct Water Decomposition on Transition Metal Surfaces: Structural Dependence and Catalytic Screening. Catalysis Letters, 2016, 146, 718-724.	1.4	18
66	Effect of Water on the CO₂ Adsorption Capacity of Amine-Functionalized Carbon Sorbents. Industrial & Engineering Chemistry Research, 2017, 56, 6317-6325.	1.8	18
67	Ab initio investigations of dioctahedral interlayer-deficient mica: modelling 1 M polymorphs of illite found within gas shale. European Journal of Mineralogy, 2014, 26, 127-144.	0.4	17
68	An electro-swing approach. Nature Energy, 2020, 5, 121-122.	19.8	15
69	Slicing the pie: how big could carbon dioxide removal be?. Wiley Interdisciplinary Reviews: Energy and Environment, 2017, 6, e253.	1.9	14
70	Experimental and Theoretical Insights into the Potential of V₂O₃ Surface Coatings for Hydrogen Permeable Vanadium Membranes. Journal of Physical Chemistry C, 2018, 122, 3488-3496.	1.5	13
71	Theoretical and experimental investigations of mercury adsorption on hematite surfaces. Journal of the Air and Waste Management Association, 2018, 68, 39-53.	0.9	13
72	Microscopic diffusion of CO 2 in clay nanopores. Chemical Physics Letters, 2017, 677, 162-166.	1.2	11

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73	Hydrogen Purification in Palladium-Based Membranes: An Operando X-ray Diffraction Study. Industrial & Engineering Chemistry Research, 2019, 58, 926-934.	1.8	11
74	Modeling CO₂ Transport and Sorption in Carbon Slit Pores. Journal of Physical Chemistry C, 2017, 121, 21018-21028.	1.5	10
75	Vanadium As a Potential Membrane Material for Carbon Capture: Effects of Minor Flue Gas Species. Environmental Science & Technology, 2017, 51, 11459-11467.	4.6	9
76	Thermochemical Analysis of Molybdenum Thin Films on Porous Alumina. Langmuir, 2017, 33, 9521-9529.	1.6	8
77	Material Consequences of Hydrogen Dissolution in Palladium Alloys Observed from First Principles. Journal of Physical Chemistry C, 2019, 123, 22158-22171.	1.5	8
78	Innovative N2-selective metallic membranes for the potential use of CO2 capture. Journal of Membrane Science, 2019, 585, 52-59.	4.1	8
79	Ab initio investigations of dioctahedral interlayer-deficient mica: Modeling particles of illite found within gas shale. American Mineralogist, 2014, 99, 1962-1972.	0.9	5
80	Theoretical Study of Nitrogen Absorption in Metals. Journal of Physical Chemistry C, 2017, 121, 17016-17028.	1.5	5
81	Design Considerations for Postcombustion CO2 Capture With Membranes. , 2018, , 385-413.		5
82	Carbon Mineralization with North American PGM Mine Tailingsâ€"Characterization and Reactivity Analysis. Minerals (Basel, Switzerland), 2021, 11, 844.	0.8	5
83	Effect of Ag and Pd promotion on CH₄selectivity in Fe(100) Fischerâ€"TrÃ¶psch catalysis. Physical Chemistry Chemical Physics, 2017, 19, 5495-5503.	1.3	4
84	Technological Pathways for Decarbonizing Petroleum Refining. , 0, , .		4
85	Dissociation, Dissolution, and Diffusion of Nitrogen on V_xFe_y and V_xCr_y Alloy Membranes Studied by First Principles. Journal of Physical Chemistry C, 2019, 123, 30416-30426.	1.5	1
86	Characterization and Adsorption Investigations of the Nanostructure of Gas Shales. , 2015, , .		0
87	Anab initiocharacterization of the electronic structure of LaCoxFe1-xO3forxâ€‰â‰‰â€‰0.5. Physica Status Solidi (B): Basic Research, 2016, 253, 1673-1687.	0.7	0
88	Assessment of the carbon abatement and removal opportunities of the Arabian Gulf Countries. Clean Energy, 2021, 5, 340-353.	1.5	0