Jennifer Wilcox

List of Publications by Year
in descending order

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	Current state of industrial heating and opportunities for decarbonization. Progress in Energy and Combustion Science, 2022, 91, 100982.	15.8	31
2	Environmental trade-offs of direct air capture technologies in climate change mitigation toward 2100. Nature Communications, 2022, 13, .	5.8	35
3	Natural Gas vs. Electricity for Solvent-Based Direct Air Capture. Frontiers in Climate, 2021, 2, .	1.3	35
4	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
5	Assessment of the carbon abatement and removal opportunities of the Arabian Gulf Countries. Clean Energy, 2021, 5, 340-353.	1.5	0
6	Carbon Mineralization with North American PGM Mine Tailingsâ€"Characterization and Reactivity Analysis. Minerals (Basel, Switzerland), 2021, 11, 844.	0.8	5
7	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
8	Ambient weathering of magnesium oxide for CO2 removal from air. Nature Communications, 2020, 11, 3299.	5.8	95
9	An electro-swing approach. Nature Energy, 2020, 5, 121-122.	19.8	15
10	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
11	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
12	Material Consequences of Hydrogen Dissolution in Palladium Alloys Observed from First Principles. Journal of Physical Chemistry C, 2019, 123, 22158-22171.	1.5	8
13	Innovative N2-selective metallic membranes for the potential use of CO2 capture. Journal of Membrane Science, 2019, 585, 52-59.	4.1	8
14	Design and operations optimization of membrane-based flexible carbon capture. International Journal of Greenhouse Gas Control, 2019, 84, 154-163.	2.3	21
15	Utilization of mineral carbonation products: current state and potential. , 2019, 9, 1096-1113.		65
16	Dissociation, Dissolution, and Diffusion of Nitrogen on V_{<i>x</i>}Fe_{<i>y</i>} and V_{<i>x</i>}Cr_{<i>y</i>} Alloy Membranes Studied by First Principles. Journal of Physical Chemistry C, 2019, 123, 30416-30426.	1.5	1
17	Hydrogen Purification in Palladium-Based Membranes: An Operando X-ray Diffraction Study. Industrial & Engineering Chemistry Research, 2019, 58, 926-934.	1.8	11
18	Idealized Shale Sorption Isotherm Measurements To Determine Pore Capacity, Pore Size Distribution, and Surface Area. Energy & Fuels, 2019, 33, 665-676.	2.5	22

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19	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
20	Carbon capture and storage (CCS): the way forward. Energy and Environmental Science, 2018, 11, 1062-1176.	15.6	2,378
21	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
22	Design Considerations for Postcombustion CO2 Capture With Membranes. , 2018, , 385-413.		5
23	Performance of Pd-Based Membranes and Effects of Various Gas Mixtures on H2 Permeation. Environments - MDPI, 2018, 5, 128.	1.5	21
24	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
25	Negative emissionsâ€"Part 1: Research landscape and synthesis. Environmental Research Letters, 2018, 13, 063001.	2.2	498
26	Thermochemical Analysis of Molybdenum Thin Films on Porous Alumina. Langmuir, 2017, 33, 9521-9529.	1.6	8
27	CO₂ Storage and Flow Capacity Measurements on Idealized Shales from Dynamic Breakthrough Experiments. Energy & Fuels, 2017, 31, 1193-1207.	2.5	38
28	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
29	Microscopic diffusion of CO 2 in clay nanopores. Chemical Physics Letters, 2017, 677, 162-166.	1.2	11
30	Effect of Water on the CO₂ Adsorption Capacity of Amine-Functionalized Carbon Sorbents. Industrial & Engineering Chemistry Research, 2017, 56, 6317-6325.	1.8	18
31	High-performance oxygen reduction and evolution carbon catalysis: From mechanistic studies to device integration. Nano Research, 2017, 10, 1163-1177.	5.8	66
32	CO 2 capture from the industry sector. Progress in Energy and Combustion Science, 2017, 63, 146-172.	15.8	247
33	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
34	Modeling CO₂ Transport and Sorption in Carbon Slit Pores. Journal of Physical Chemistry C, 2017, 121, 21018-21028.	1.5	10
35	Carbon Capture and Utilization in the Industrial Sector. Environmental Science & Technology, 2017, 51, 11440-11449.	4.6	91
36	Theoretical Study of Nitrogen Absorption in Metals. Journal of Physical Chemistry C, 2017, 121, 17016-17028.	1.5	5

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37	Selection of Shale Preparation Protocol and Outgas Procedures for Applications in Low-Pressure Analysis. Energy & Fuels, 2017, 31, 9043-9051.	2.5	60
38	Slicing the pie: how big could carbon dioxide removal be?. Wiley Interdisciplinary Reviews: Energy and Environment, 2017, 6, e253.	1.9	14
39	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
40	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
41	Supported Pd-Au Membrane Reactor for Hydrogen Production: Membrane Preparation, Characterization and Testing. Molecules, 2016, 21, 581.	1.7	29
42	Tunable Polyanilineâ€Based Porous Carbon with Ultrahigh Surface Area for CO₂ Capture at Elevated Pressure. Advanced Energy Materials, 2016, 6, 1502491.	10.2	129
43	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
44	Molecular simulations of nitrogen-doped hierarchical carbon adsorbents for post-combustion CO₂ capture. Physical Chemistry Chemical Physics, 2016, 18, 28747-28758.	1.3	21
45	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
46	Direct Water Decomposition on Transition Metal Surfaces: Structural Dependence and Catalytic Screening. Catalysis Letters, 2016, 146, 718-724.	1.4	18
47	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
48	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
49	Characterization and Adsorption Investigations of the Nanostructure of Gas Shales. , 2015, , .		0
50	Ultrahigh Surface Area Three-Dimensional Porous Graphitic Carbon from Conjugated Polymeric Molecular Framework. ACS Central Science, 2015, 1, 68-76.	5.3	207
51	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
52	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
53	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
54	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

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55	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
56	Klinkenberg effect on predicting and measuring helium permeability in gas shales. International Journal of Coal Geology, 2014, 123, 62-68.	1.9	125
57	Revisiting film theory to consider approaches for enhanced solvent-process design for carbon capture. Energy and Environmental Science, 2014, 7, 1769.	15.6	34
58	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
59	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
60	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
61	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
62	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
63	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
64	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
65	Heterogeneous Mercury Oxidation on Au(111) from First Principles. Environmental Science & Technology, 2013, 47, 8515-8522.	4.6	103
66	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
67	Impact of alkalinity sources on the life-cycle energy efficiency of mineral carbonation technologies. Energy and Environmental Science, 2012, 5, 8631.	15.6	64
68	Investigation of Adsorption Behavior of Mercury on Au(111) from First Principles. Environmental Science & Technology, 2012, 46, 7260-7266.	4.6	51
69	Effects of Surface Heterogeneity on the Adsorption of CO₂ in Microporous Carbons. Environmental Science & Technology, 2012, 46, 1940-1947.	4.6	243
70	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
71	Carbon Capture. , 2012, , .		144
72	Mercury adsorption and oxidation in coal combustion and gasification processes. International Journal of Coal Geology, 2012, 90-91, 4-20.	1.9	251

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73	Molecular modeling of carbon dioxide transport and storage in porous carbon-based materials. Microporous and Mesoporous Materials, 2012, 158, 195-203.	2.2	79
74	Heterogeneous Mercury Reaction Chemistry on Activated Carbon. Journal of the Air and Waste Management Association, 2011, 61, 418-426.	0.9	80
75	Ab initio-based Mercury Oxidation Kinetics via Bromine at Postcombustion Flue Gas Conditions. Energy & Fuels, 2011, 25, 1348-1356.	2.5	30
76	CO₂Adsorption on Carbon Models of Organic Constituents of Gas Shale and Coal. Environmental Science & Technology, 2011, 45, 809-814.	4.6	163
77	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
78	DFT-Based Study on Oxygen Adsorption on Defective Graphene-Supported Pt Nanoparticles. Journal of Physical Chemistry C, 2011, 115, 22742-22747.	1.5	200
79	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 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
80	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
81	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<m xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î±</m Physic	1.1	26
82	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
83	Hg Binding on Pd Binary Alloys and Overlays. Journal of Physical Chemistry C, 2009, 113, 7813-7820.	1.5	49
84	A Kinetic Investigation of High-Temperature Mercury Oxidation by Chlorine. Journal of Physical Chemistry A, 2009, 113, 6633-6639.	1.1	50
85	Mercury Species and SO₂ Adsorption on CaO(100). Journal of Physical Chemistry C, 2008, 112, 16484-16490.	1.5	73
86	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
87	Mercury binding on activated carbon. Environmental Progress, 2006, 25, 319-326.	0.8	101
88	Technological Pathways for Decarbonizing Petroleum Refining. , 0, , .		4