

Li-Chiang Lin

List of Publications by Year in descending order

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98
papers

6,000
citations

94269

37
h-index

74018

75
g-index

104
all docs

104
docs citations

104
times ranked

6492
citing authors

#	ARTICLE	IF	CITATIONS
1	Robust ultrathin nanoporous MOF membrane with intra-crystalline defects for fast water transport. <i>Nature Communications</i> , 2022, 13, 266.	5.8	76
2	New sterically hindered polyvinylamine-containing membranes for CO ₂ capture from flue gas. <i>Journal of Membrane Science</i> , 2022, 645, 120195.	4.1	12
3	Chemistry-Encoded Convolutional Neural Networks for Predicting Gaseous Adsorption in Porous Materials. <i>Journal of Physical Chemistry C</i> , 2022, 126, 2813-2822.	1.5	19
4	Scalable robust nano-porous Zr-based MOF adsorbent with high-capacity for sustainable water purification. <i>Separation and Purification Technology</i> , 2022, 288, 120620.	3.9	32
5	Computational Prediction of Water Sorption in Facilitated Transport Membranes. <i>Journal of Physical Chemistry C</i> , 2022, 126, 3661-3670.	1.5	9
6	Responses to the comments on "Monte Carlo simulations for water adsorption in porous materials: Best practices and new insights". <i>AIChE Journal</i> , 2022, 68, .	1.8	3
7	Superhydrophobic Carbon Nanotube Network Membranes for Membrane Distillation: High-Throughput Performance and Transport Mechanism. <i>Environmental Science & Technology</i> , 2022, 56, 5775-5785.	4.6	21
8	Deep learning neural network potential for simulating gaseous adsorption in metal-organic frameworks. <i>Materials Advances</i> , 2022, 3, 5299-5303.	2.6	4
9	Computational Study of Alkane Adsorption in Brønsted Acid Zeolites for More Efficient Alkane Cracking. <i>Langmuir</i> , 2022, 38, 7665-7677.	1.6	2
10	A new measurement of amine steric hindrance N exposure. <i>Separation and Purification Technology</i> , 2022, 299, 121601.	3.9	4
11	Highly CO ₂ Selective Metal-Organic Framework Membranes with Favorable Coulombic Effect. <i>Advanced Functional Materials</i> , 2021, 31, 2006924.	7.8	42
12	Improving Computational Assessment of Porous Materials for Water Adsorption Applications via Flat Histogram Methods. <i>Journal of Physical Chemistry C</i> , 2021, 125, 4253-4266.	1.5	16
13	Nanoporous Material Recognition via 3D Convolutional Neural Networks: Prediction of Adsorption Properties. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2279-2285.	2.1	22
14	A flame-retardant post-synthetically functionalized COF sponge as absorbent for spilled oil recovery. <i>Journal of Materials Science</i> , 2021, 56, 13031.	1.7	6
15	Facile Defect Engineering of Zeolitic Imidazolate Frameworks towards Enhanced C ₃ H ₆ /C ₃ H ₈ Separation Performance. <i>Advanced Functional Materials</i> , 2021, 31, 2105577.	7.8	26
16	Suppressing Defect Formation in Metal-Organic Framework Membranes via Plasma-Assisted Synthesis for Gas Separations. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 41904-41915.	4.0	23
17	Transport-Relevant Pore Limiting Diameter for Molecular Separations in Metal-Organic Framework Membranes. <i>Journal of Physical Chemistry C</i> , 2021, 125, 20416-20425.	1.5	6
18	Solubility selectivity-enhanced SIFSIX-3-Ni-containing mixed matrix membranes for improved CO ₂ /CH ₄ separation efficiency. <i>Journal of Membrane Science</i> , 2021, 633, 119390.	4.1	13

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19	Toward Sustainable Metal-Organic Frameworks for Post-Combustion Carbon Capture by Life Cycle Assessment and Molecular Simulation. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 12132-12141.	3.2	10
20	Monte Carlo simulations for water adsorption in porous materials: Best practices and new insights. <i>AIChE Journal</i> , 2021, 67, e17447.	1.8	19
21	Pillared-bilayer metal-organic framework membranes for dehydration of isopropanol. <i>Microporous and Mesoporous Materials</i> , 2021, 326, 111344.	2.2	15
22	NaP1 zeolite membranes with high selectivity for water-alcohol pervaporation. <i>Journal of Membrane Science</i> , 2021, 639, 119762.	4.1	18
23	Coulombic effect on permeation of CO ₂ in metal-organic framework membranes. <i>Journal of Membrane Science</i> , 2021, 639, 119742.	4.1	23
24	In Silico Screening of Zeolites for the Highly Selective Adsorption of Central C-C Bonds toward More Effective Alkane Cracking. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 15174-15183.	1.8	2
25	Fundamental Insights on Hydration Environment of Boric Acid and Its Role in Separation from Saline Water. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1438-1445.	1.5	35
26	Machine Learning-Aided Computational Study of Metal-Organic Frameworks for Sour Gas Sweetening. <i>Journal of Physical Chemistry C</i> , 2020, 124, 27580-27591.	1.5	29
27	Exploiting interior surface functionalization in reverse osmosis desalination membranes to mitigate permeability-selectivity trade-off: Molecular simulations of nanotube-based membranes. <i>Desalination</i> , 2020, 491, 114537.	4.0	17
28	Toward Long-Lasting Low-Haze Antifog Coatings through the Deposition of Zeolites. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 13042-13050.	1.8	8
29	Beyond the BET Analysis: The Surface Area Prediction of Nanoporous Materials Using a Machine Learning Method. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 5412-5417.	2.1	37
30	Potential and Design of Zeolite Nanosheets as Pervaporation Membranes for Ethanol Extraction. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 12845-12854.	1.8	12
31	Efficient and Accurate Charge Assignments via a Multilayer Connectivity-Based Atom Contribution (m-CBAC) Approach. <i>Journal of Physical Chemistry C</i> , 2020, 124, 11428-11437.	1.5	21
32	Computational Evaluation of Carriers in Facilitated Transport Membranes for Postcombustion Carbon Capture. <i>Journal of Physical Chemistry C</i> , 2020, 124, 25322-25330.	1.5	25
33	Surface Area Determination of Porous Materials Using the Brunauer-Emmett-Teller (BET) Method: Limitations and Improvements. <i>Journal of Physical Chemistry C</i> , 2019, 123, 20195-20209.	1.5	130
34	Electrostatic Potential Optimized Molecular Models for Molecular Simulations: CO, CO ₂ , COS, H ₂ S, N ₂ , N ₂ O, and SO ₂ . <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6323-6332.	2.3	12
35	Activation-Controlled Structure Deformation of Pillared-Bilayer Metal-Organic Framework Membranes for Gas Separations. <i>Chemistry of Materials</i> , 2019, 31, 7666-7677.	3.2	32
36	Exploring the Potential of Defective UiO-66 as Reverse Osmosis Membranes for Desalination. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16118-16126.	1.5	35

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37	Computational discovery of nanoporous materials for energy- and environment-related applications. <i>Molecular Simulation</i> , 2019, 45, 1122-1147.	0.9	23
38	Excimer-Mediated Intermolecular Charge Transfer in Self-Assembled Donor-acceptor Dyes on Metal Oxides. <i>Journal of the American Chemical Society</i> , 2019, 141, 8727-8731.	6.6	22
39	Response to "Impact of Zeolite Structure on Entropic/Enthalpic Contributions to Alkane Monomolecular Cracking: An IR Operando Study". <i>Chemistry - A European Journal</i> , 2019, 25, 7225-7226.	1.7	1
40	Decoupling pH Dependence of Flat Band Potential in Aqueous Dye-Sensitized Electrodes. <i>Journal of Physical Chemistry C</i> , 2019, 123, 8681-8687.	1.5	17
41	Aggregation Behavior of Inorganic 2D Nanomaterials Beyond Graphene: Insights from Molecular Modeling and Modified DLVO Theory. <i>Environmental Science & Technology</i> , 2019, 53, 4161-4172.	4.6	51
42	Hexagonal Superalignment of Nano-Objects with Tunable Separation in a Dilute and Spacer-Free Solution. <i>Physical Review Letters</i> , 2019, 123, 238002.	2.9	10
43	Role of Structural Defects in the Water Adsorption Properties of MOF-801. <i>Journal of Physical Chemistry C</i> , 2018, 122, 5545-5552.	1.5	68
44	Understanding Brønsted-Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. <i>ChemPhysChem</i> , 2018, 19, 338-338.	1.0	0
45	Transferability of CO ₂ Force Fields for Prediction of Adsorption Properties in All-Silica Zeolites. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10892-10903.	1.5	12
46	Atomistic Investigations of the Effects of Si/Al Ratio and Al Distribution on the Adsorption Selectivity of <i>n</i> -Alkanes in Brønsted-Acid Zeolites. <i>Journal of Physical Chemistry C</i> , 2018, 122, 9397-9410.	1.5	35
47	Investigation of the Water Adsorption Properties and Structural Stability of MIL-100(Fe) with Different Anions. <i>Langmuir</i> , 2018, 34, 4180-4187.	1.6	33
48	Understanding Brønsted-Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. <i>ChemPhysChem</i> , 2018, 19, 341-358.	1.0	21
49	Potential of polarizable force fields for predicting the separation performance of small hydrocarbons in M-MOF-74. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28848-28859.	1.3	18
50	Frontispiece: Tuning Gas Adsorption by Metal Node Blocking in Photoresponsive Metal-Organic Frameworks. <i>Chemistry - A European Journal</i> , 2018, 24, .	1.7	0
51	Bioinspired Metal-Organic Framework for Trace CO ₂ Capture. <i>Journal of the American Chemical Society</i> , 2018, 140, 12662-12666.	6.6	132
52	Exploring the potential and design of zeolite nanosheets as pervaporation membranes for ethanol extraction. <i>Chemical Communications</i> , 2018, 54, 13200-13203.	2.2	13
53	Polarizable Force Field for CO ₂ in M-MOF-74 Derived from Quantum Mechanics. <i>Journal of Physical Chemistry C</i> , 2018, 122, 24488-24498.	1.5	29
54	Systematic molecular model development with reliable charge distributions for gaseous adsorption in nanoporous materials. <i>Journal of Materials Chemistry A</i> , 2018, 6, 16029-16042.	5.2	12

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55	Rational Design of Two-Dimensional Hydrocarbon Polymer as Ultrathin-Film Nanoporous Membranes for Water Desalination. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 18778-18786.	4.0	31
56	Tuning Gas Adsorption by Metal Node Blocking in Photoresponsive Metal-Organic Frameworks. <i>Chemistry - A European Journal</i> , 2018, 24, 15167-15172.	1.7	33
57	Polarizable Force Fields for CO ₂ and CH ₄ Adsorption in M-MOF-74. <i>Journal of Physical Chemistry C</i> , 2017, 121, 4659-4673.	1.5	87
58	Theoretical Analysis of the Influence of Pore Geometry on Monomolecular Cracking and Dehydrogenation of n-Butane in Brønsted Acidic Zeolites. <i>ACS Catalysis</i> , 2017, 7, 2685-2697.	5.5	42
59	Understanding gas adsorption in MOF-5/graphene oxide composite materials. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 11639-11644.	1.3	24
60	Atomistic Understanding of Zeolite Nanosheets for Water Desalination. <i>Journal of Physical Chemistry C</i> , 2017, 121, 11273-11280.	1.5	60
61	Effects of Pore and Cage Topology on the Thermodynamics of n-Alkane Adsorption at Brønsted Protons in Zeolites at High Temperature. <i>Journal of Physical Chemistry C</i> , 2017, 121, 1618-1638.	1.5	17
62	Investigating the Potential of Single-Walled Aluminosilicate Nanotubes in Water Desalination. <i>ChemPhysChem</i> , 2017, 18, 179-183.	1.0	26
63	Atomistic understanding of cation exchange in PbS nanocrystals using simulations with pseudoligands. <i>Nature Communications</i> , 2016, 7, 11503.	5.8	48
64	Investigating polarization effects of CO ₂ adsorption in MgMOF-74. <i>Journal of Computational Science</i> , 2016, 15, 86-94.	1.5	25
65	Force Field Development from Periodic Density Functional Theory Calculations for Gas Separation Applications Using Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2016, 120, 12590-12604.	1.5	95
66	High-throughput computational screening of nanoporous adsorbents for CO ₂ capture from natural gas. <i>Molecular Systems Design and Engineering</i> , 2016, 1, 175-188.	1.7	54
67	Assessing the Surface Area of Porous Solids: Limitations, Probe Molecules, and Methods. <i>Langmuir</i> , 2016, 32, 12664-12675.	1.6	33
68	Multilayer Nanoporous Graphene Membranes for Water Desalination. <i>Nano Letters</i> , 2016, 16, 1027-1033.	4.5	331
69	Effects of Zeolite Structural Confinement on Adsorption Thermodynamics and Reaction Kinetics for Monomolecular Cracking and Dehydrogenation of n-Butane. <i>Journal of the American Chemical Society</i> , 2016, 138, 4739-4756.	6.6	72
70	Nanoporous Materials Can Tune the Critical Point of a Pure Substance. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 14349-14352.	7.2	16
71	Adsorption Thermodynamics and Intrinsic Activation Parameters for Monomolecular Cracking of n-Alkanes on Brønsted Acid Sites in Zeolites. <i>Journal of Physical Chemistry C</i> , 2015, 119, 10427-10438.	1.5	48
72	Water adsorption in metal-organic frameworks with open-metal sites. <i>AIChE Journal</i> , 2015, 61, 677-687.	1.8	37

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73	Small-Molecule Adsorption in Open-Site Metal-Organic Frameworks: A Systematic Density Functional Theory Study for Rational Design. <i>Chemistry of Materials</i> , 2015, 27, 668-678.	3.2	248
74	Atomistic understandings of reduced graphene oxide as an ultrathin-film nanoporous membrane for separations. <i>Nature Communications</i> , 2015, 6, 8335.	5.8	214
75	Two-dimensional covalent triazine framework as an ultrathin-film nanoporous membrane for desalination. <i>Chemical Communications</i> , 2015, 51, 14921-14924.	2.2	127
76	Metal-Organic Frameworks in Adsorption-Driven Heat Pumps: The Potential of Alcohols as Working Fluids. <i>Langmuir</i> , 2015, 31, 12783-12796.	1.6	123
77	Computational screening of porous metal-organic frameworks and zeolites for the removal of SO ₂ and NO _x from flue gases. <i>AIChE Journal</i> , 2014, 60, 2314-2323.	1.8	112
78	Design of a Metal-Organic Framework with Enhanced Back Bonding for Separation of N ₂ and CH ₄ . <i>Journal of the American Chemical Society</i> , 2014, 136, 698-704.	6.6	157
79	A hybrid absorption-adsorption method to efficiently capture carbon. <i>Nature Communications</i> , 2014, 5, 5147.	5.8	163
80	Optimizing nanoporous materials for gas storage. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 5499.	1.3	76
81	Efficient Determination of Accurate Force Fields for Porous Materials Using ab Initio Total Energy Calculations. <i>Journal of Physical Chemistry C</i> , 2014, 118, 2693-2701.	1.5	23
82	Evaluating different classes of porous materials for carbon capture. <i>Energy and Environmental Science</i> , 2014, 7, 4132-4146.	15.6	186
83	CO ₂ Adsorption in Fe ₂ (dobdc): A Classical Force Field Parameterized from Quantum Mechanical Calculations. <i>Journal of Physical Chemistry C</i> , 2014, 118, 12230-12240.	1.5	45
84	Force-Field Development from Electronic Structure Calculations with Periodic Boundary Conditions: Applications to Gaseous Adsorption and Transport in Metal-Organic Frameworks. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1477-1488.	2.3	121
85	Reversible CO Binding Enables Tunable CO/H ₂ and CO/N ₂ Separations in Metal-Organic Frameworks with Exposed Divalent Metal Cations. <i>Journal of the American Chemical Society</i> , 2014, 136, 10752-10761.	6.6	210
86	Methane storage capabilities of diamond analogues. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 20937.	1.3	10
87	Evaluating mixture adsorption models using molecular simulation. <i>AIChE Journal</i> , 2013, 59, 3054-3064.	1.8	31
88	New materials for methane capture from dilute and medium-concentration sources. <i>Nature Communications</i> , 2013, 4, 1694.	5.8	111
89	Understanding CO ₂ Dynamics in Metal-Organic Frameworks with Open Metal Sites. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 4410-4413.	7.2	160
90	Large-Scale Screening of Zeolite Structures for CO ₂ Membrane Separations. <i>Journal of the American Chemical Society</i> , 2013, 135, 7545-7552.	6.6	105

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91	The Mechanism of Carbon Dioxide Adsorption in an Alkylamine-Functionalized Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2013, 135, 7402-7405.	6.6	208
92	Mail-Order Metal-Organic Frameworks (MOFs): Designing Isoreticular MOF-5 Analogues Comprising Commercially Available Organic Molecules. <i>Journal of Physical Chemistry C</i> , 2013, 117, 12159-12167.	1.5	64
93	Innenrücktitelbild: Understanding CO ₂ Dynamics in Metal-Organic Frameworks with Open Metal Sites (<i>Angew. Chem.</i> 16/2013). <i>Angewandte Chemie</i> , 2013, 125, 4589-4589.	1.6	0
94	Predicting Large CO ₂ Adsorption in Aluminosilicate Zeolites for Postcombustion Carbon Dioxide Capture. <i>Journal of the American Chemical Society</i> , 2012, 134, 18940-18943.	6.6	129
95	Ab initio carbon capture in open-site metal-organic frameworks. <i>Nature Chemistry</i> , 2012, 4, 810-816.	6.6	310
96	Similarity-Driven Discovery of Zeolite Materials for Adsorption-Based Separations. <i>ChemPhysChem</i> , 2012, 13, 3595-3597.	1.0	43
97	In silico screening of carbon-capture materials. <i>Nature Materials</i> , 2012, 11, 633-641.	13.3	497
98	Large-Scale Computational Screening of Zeolites for Ethane/Ethene Separation. <i>Langmuir</i> , 2012, 28, 11914-11919.	1.6	90