Li-Chiang Lin

List of Publications by Year
in descending order

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98	6,000	94381	74108
papers	citations	37 h-index	75 g-index

104	104	104	6492
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	In silico screening of carbon-capture materials. Nature Materials, 2012, 11, 633-641.	13.3	497
2	Multilayer Nanoporous Graphene Membranes for Water Desalination. Nano Letters, 2016, 16, 1027-1033.	4.5	331
3	Ab initio carbon capture in open-site metalâ€“organic frameworks. Nature Chemistry, 2012, 4, 810-816.	6.6	310
4	Small-Molecule Adsorption in Open-Site Metalâ€“Organic Frameworks: A Systematic Density Functional Theory Study for Rational Design. Chemistry of Materials, 2015, 27, 668-678.	3.2	248
5	Atomistic understandings of reduced graphene oxide as an ultrathin-film nanoporous membrane for separations. Nature Communications, 2015, 6, 8335.	5.8	214
6	Reversible CO Binding Enables Tunable CO/H₂ and CO/N₂ Separations in Metalâ€“Organic Frameworks with Exposed Divalent Metal Cations. Journal of the American Chemical Society, 2014, 136, 10752-10761.	6.6	210
7	The Mechanism of Carbon Dioxide Adsorption in an Alkylamine-Functionalized Metalâ€“Organic Framework. Journal of the American Chemical Society, 2013, 135, 7402-7405.	6.6	208
8	Evaluating different classes of porous materials for carbon capture. Energy and Environmental Science, 2014, 7, 4132-4146.	15.6	186
9	A hybrid absorptionâ€“adsorption method to efficiently capture carbon. Nature Communications, 2014, 5, 5147.	5.8	163
10	Understanding CO₂ Dynamics in Metalâ€“Organic Frameworks with Open Metal Sites. Angewandte Chemie - International Edition, 2013, 52, 4410-4413.	7.2	160
11	Design of a Metalâ€“Organic Framework with Enhanced Back Bonding for Separation of N₂ and CH₄. Journal of the American Chemical Society, 2014, 136, 698-704.	6.6	157
12	Bioinspired Metalâ€“Organic Framework for Trace CO₂ Capture. Journal of the American Chemical Society, 2018, 140, 12662-12666.	6.6	132
13	Surface Area Determination of Porous Materials Using the Brunauerâ€“Emmettâ€“Teller (BET) Method: Limitations and Improvements. Journal of Physical Chemistry C, 2019, 123, 20195-20209.	1.5	130
14	Predicting Large CO₂ Adsorption in Aluminosilicate Zeolites for Postcombustion Carbon Dioxide Capture. Journal of the American Chemical Society, 2012, 134, 18940-18943.	6.6	129
15	Two-dimensional covalent triazine framework as an ultrathin-film nanoporous membrane for desalination. Chemical Communications, 2015, 51, 14921-14924.	2.2	127
16	Metalâ€“Organic Frameworks in Adsorption-Driven Heat Pumps: The Potential of Alcohols as Working Fluids. Langmuir, 2015, 31, 12783-12796.	1.6	123
17	Force-Field Development from Electronic Structure Calculations with Periodic Boundary Conditions: Applications to Gaseous Adsorption and Transport in Metalâ€“Organic Frameworks. Journal of Chemical Theory and Computation, 2014, 10, 1477-1488.	2.3	121
18	Computational screening of porous metalâ€organic frameworks and zeolites for the removal of SO₂ and NO_x from flue gases. AICHE Journal, 2014, 60, 2314-2323.	1.8	112

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19	New materials for methane capture from dilute and medium-concentration sources. Nature Communications, 2013, 4, 1694.	5.8	111
20	Large-Scale Screening of Zeolite Structures for CO₂ Membrane Separations. Journal of the American Chemical Society, 2013, 135, 7545-7552.	6.6	105
21	Force Field Development from Periodic Density Functional Theory Calculations for Gas Separation Applications Using Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2016, 120, 12590-12604.	1.5	95
22	Large-Scale Computational Screening of Zeolites for Ethane/Ethene Separation. Langmuir, 2012, 28, 11914-11919.	1.6	90
23	Polarizable Force Fields for CO₂ and CH₄ Adsorption in M-MOF-74. Journal of Physical Chemistry C, 2017, 121, 4659-4673.	1.5	87
24	Optimizing nanoporous materials for gas storage. Physical Chemistry Chemical Physics, 2014, 16, 5499.	1.3	76
25	Robust ultrathin nanoporous MOF membrane with intra-crystalline defects for fast water transport. Nature Communications, 2022, 13, 266.	5.8	76
26	Effects of Zeolite Structural Confinement on Adsorption Thermodynamics and Reaction Kinetics for Monomolecular Cracking and Dehydrogenation of n-Butane. Journal of the American Chemical Society, 2016, 138, 4739-4756.	6.6	72
27	Role of Structural Defects in the Water Adsorption Properties of MOF-801. Journal of Physical Chemistry C, 2018, 122, 5545-5552.	1.5	68
28	Mail-Order Metalâ€“Organic Frameworks (MOFs): Designing Isoreticular MOF-5 Analogues Comprising Commercially Available Organic Molecules. Journal of Physical Chemistry C, 2013, 117, 12159-12167.	1.5	64
29	Atomistic Understanding of Zeolite Nanosheets for Water Desalination. Journal of Physical Chemistry C, 2017, 121, 11273-11280.	1.5	60
30	High-throughput computational screening of nanoporous adsorbents for CO₂ capture from natural gas. Molecular Systems Design and Engineering, 2016, 1, 175-188.	1.7	54
31	Aggregation Behavior of Inorganic 2D Nanomaterials Beyond Graphene: Insights from Molecular Modeling and Modified DLVO Theory. Environmental Science & Technology, 2019, 53, 4161-4172.	4.6	51
32	Adsorption Thermodynamics and Intrinsic Activation Parameters for Monomolecular Cracking of n-Alkanes on BrÃ¸nsted Acid Sites in Zeolites. Journal of Physical Chemistry C, 2015, 119, 10427-10438.	1.5	48
33	Atomistic understanding of cation exchange in PbS nanocrystals using simulations with pseudoligands. Nature Communications, 2016, 7, 11503.	5.8	48
34	CO₂ Adsorption in Fe₂(dobdc): A Classical Force Field Parameterized from Quantum Mechanical Calculations. Journal of Physical Chemistry C, 2014, 118, 12230-12240.	1.5	45
35	Similarityâ€Driven Discovery of Zeolite Materials for Adsorptionâ€Based Separations. ChemPhysChem, 2012, 13, 3595-3597.	1.0	43
36	Theoretical Analysis of the Influence of Pore Geometry on Monomolecular Cracking and Dehydrogenation ofn-Butane in BrÃ¸nsted Acidic Zeolites. ACS Catalysis, 2017, 7, 2685-2697.	5.5	42

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37	Highly CO₂ Selective Metalâ€“Organic Framework Membranes with Favorable Coulombic Effect. Advanced Functional Materials, 2021, 31, 2006924.	7.8	42
38	Water adsorption in metalâ€“organic frameworks with openâ€metal sites. AICHE Journal, 2015, 61, 677-687.	1.8	37
39	Beyond the BET Analysis: The Surface Area Prediction of Nanoporous Materials Using a Machine Learning Method. Journal of Physical Chemistry Letters, 2020, 11, 5412-5417.	2.1	37
40	Atomistic Investigations of the Effects of Si/Al Ratio and Al Distribution on the Adsorption Selectivity of n-Alkanes in BrÃ¸nsted-Acid Zeolites. Journal of Physical Chemistry C, 2018, 122, 9397-9410.	1.5	35
41	Exploring the Potential of Defective UiO-66 as Reverse Osmosis Membranes for Desalination. Journal of Physical Chemistry C, 2019, 123, 16118-16126.	1.5	35
42	Fundamental Insights on Hydration Environment of Boric Acid and Its Role in Separation from Saline Water. Journal of Physical Chemistry C, 2020, 124, 1438-1445.	1.5	35
43	Assessing the Surface Area of Porous Solids: Limitations, Probe Molecules, and Methods. Langmuir, 2016, 32, 12664-12675.	1.6	33
44	Investigation of the Water Adsorption Properties and Structural Stability of MIL-100(Fe) with Different Anions. Langmuir, 2018, 34, 4180-4187.	1.6	33
45	Tuning Gas Adsorption by Metal Node Blocking in Photoresponsive Metalâ€“Organic Frameworks. Chemistry - A European Journal, 2018, 24, 15167-15172.	1.7	33
46	Activation-Controlled Structure Deformation of Pillared-Bilayer Metalâ€“Organic Framework Membranes for Gas Separations. Chemistry of Materials, 2019, 31, 7666-7677.	3.2	32
47	Scalable robust nano-porous Zr-based MOF adsorbent with high-capacity for sustainable water purification. Separation and Purification Technology, 2022, 288, 120620.	3.9	32
48	Evaluating mixture adsorption models using molecular simulation. AICHE Journal, 2013, 59, 3054-3064.	1.8	31
49	Rational Design of Two-Dimensional Hydrocarbon Polymer as Ultrathin-Film Nanoporous Membranes for Water Desalination. ACS Applied Materials & Interfaces, 2018, 10, 18778-18786.	4.0	31
50	Polarizable Force Field for CO₂ in M-MOF-74 Derived from Quantum Mechanics. Journal of Physical Chemistry C, 2018, 122, 24488-24498.	1.5	29
51	Machine Learning-Aided Computational Study of Metalâ€“Organic Frameworks for Sour Gas Sweetening. Journal of Physical Chemistry C, 2020, 124, 27580-27591.	1.5	29
52	Investigating the Potential of Singleâ€Walled Aluminosilicate Nanotubes in Water Desalination. ChemPhysChem, 2017, 18, 179-183.	1.0	26
53	Facile Defect Engineering of Zeolitic Imidazolate Frameworks towards Enhanced C₃H₆/C₃H₈ Separation Performance. Advanced Functional Materials, 2021, 31, 2105577.	7.8	26
54	Investigating polarization effects of CO2 adsorption in MgMOF-74. Journal of Computational Science, 2016, 15, 86-94.	1.5	25

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55	Computational Evaluation of Carriers in Facilitated Transport Membranes for Postcombustion Carbon Capture. Journal of Physical Chemistry C, 2020, 124, 25322-25330.	1.5	25
56	Understanding gas adsorption in MOF-5/graphene oxide composite materials. Physical Chemistry Chemical Physics, 2017, 19, 11639-11644.	1.3	24
57	Efficient Determination of Accurate Force Fields for Porous Materials Using ab Initio Total Energy Calculations. Journal of Physical Chemistry C, 2014, 118, 2693-2701.	1.5	23
58	Computational discovery of nanoporous materials for energy- and environment-related applications. Molecular Simulation, 2019, 45, 1122-1147.	0.9	23
59	Suppressing Defect Formation in Metalâ€“Organic Framework Membranes via Plasma-Assisted Synthesis for Gas Separations. ACS Applied Materials & Interfaces, 2021, 13, 41904-41915.	4.0	23
60	Coulombic effect on permeation of CO2 in metal-organic framework membranes. Journal of Membrane Science, 2021, 639, 119742.	4.1	23
61	Excimer-Mediated Intermolecular Charge Transfer in Self-Assembled Donorâ€“Acceptor Dyes on Metal Oxides. Journal of the American Chemical Society, 2019, 141, 8727-8731.	6.6	22
62	Nanoporous Material Recognition via 3D Convolutional Neural Networks: Prediction of Adsorption Properties. Journal of Physical Chemistry Letters, 2021, 12, 2279-2285.	2.1	22
63	Understanding BrÃ¸nstedâ€Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. ChemPhysChem, 2018, 19, 341-358.	1.0	21
64	Efficient and Accurate Charge Assignments via a Multilayer Connectivity-Based Atom Contribution (m-CBAC) Approach. Journal of Physical Chemistry C, 2020, 124, 11428-11437.	1.5	21
65	Superhydrophobic Carbon Nanotube Network Membranes for Membrane Distillation: High-Throughput Performance and Transport Mechanism. Environmental Science & Technology, 2022, 56, 5775-5785.	4.6	21
66	Monte Carlo simulations for water adsorption in porous materials: Best practices and new insights. AICHE Journal, 2021, 67, e17447.	1.8	19
67	Chemistry-Encoded Convolutional Neural Networks for Predicting Gaseous Adsorption in Porous Materials. Journal of Physical Chemistry C, 2022, 126, 2813-2822.	1.5	19
68	Potential of polarizable force fields for predicting the separation performance of small hydrocarbons in M-MOF-74. Physical Chemistry Chemical Physics, 2018, 20, 28848-28859.	1.3	18
69	NaP1 zeolite membranes with high selectivity for water-alcohol pervaporation. Journal of Membrane Science, 2021, 639, 119762.	4.1	18
70	Effects of Pore and Cage Topology on the Thermodynamics of n-Alkane Adsorption at BrÃ¸nsted Protons in Zeolites at High Temperature. Journal of Physical Chemistry C, 2017, 121, 1618-1638.	1.5	17
71	Decoupling pH Dependence of Flat Band Potential in Aqueous Dye-Sensitized Electrodes. Journal of Physical Chemistry C, 2019, 123, 8681-8687.	1.5	17
72	Exploiting interior surface functionalization in reverse osmosis desalination membranes to mitigate permeabilityâ€“selectivity trade-off: Molecular simulations of nanotube-based membranes. Desalination, 2020, 491, 114537.	4.0	17

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73	Nanoporous Materials Can Tune the Critical Point of a Pure Substance. Angewandte Chemie - International Edition, 2015, 54, 14349-14352.	7.2	16
74	Improving Computational Assessment of Porous Materials for Water Adsorption Applications via Flat Histogram Methods. Journal of Physical Chemistry C, 2021, 125, 4253-4266.	1.5	16
75	Pillared-bilayer metal-organic framework membranes for dehydration of isopropanol. Microporous and Mesoporous Materials, 2021, 326, 111344.	2.2	15
76	Exploring the potential and design of zeolite nanosheets as pervaporation membranes for ethanol extraction. Chemical Communications, 2018, 54, 13200-13203.	2.2	13
77	Solubility selectivity-enhanced SIFSIX-3-Ni-containing mixed matrix membranes for improved CO2/CH4 separation efficiency. Journal of Membrane Science, 2021, 633, 119390.	4.1	13
78	Transferability of CO₂ Force Fields for Prediction of Adsorption Properties in All-Silica Zeolites. Journal of Physical Chemistry C, 2018, 122, 10892-10903.	1.5	12
79	Systematic molecular model development with reliable charge distributions for gaseous adsorption in nanoporous materials. Journal of Materials Chemistry A, 2018, 6, 16029-16042.	5.2	12
80	Electrostatic Potential Optimized Molecular Models for Molecular Simulations: CO, CO2, COS, H2S, N2, N2O, and SO2. Journal of Chemical Theory and Computation, 2019, 15, 6323-6332.	2.3	12
81	Potential and Design of Zeolite Nanosheets as Pervaporation Membranes for Ethanol Extraction. Industrial & Engineering Chemistry Research, 2020, 59, 12845-12854.	1.8	12
82	New sterically hindered polyvinylamine-containing membranes for CO2 capture from flue gas. Journal of Membrane Science, 2022, 645, 120195.	4.1	12
83	Methane storage capabilities of diamond analogues. Physical Chemistry Chemical Physics, 2013, 15, 20937.	1.3	10
84	Hexagonal Superalignment of Nano-Objects with Tunable Separation in a Dilute and Spacer-Free Solution. Physical Review Letters, 2019, 123, 238002.	2.9	10
85	Toward Sustainable Metalâ€“Organic Frameworks for Post-Combustion Carbon Capture by Life Cycle Assessment and Molecular Simulation. ACS Sustainable Chemistry and Engineering, 2021, 9, 12132-12141.	3.2	10
86	Computational Prediction of Water Sorption in Facilitated Transport Membranes. Journal of Physical Chemistry C, 2022, 126, 3661-3670.	1.5	9
87	Toward Long-Lasting Low-Haze Antifog Coatings through the Deposition of Zeolites. Industrial & Engineering Chemistry Research, 2020, 59, 13042-13050.	1.8	8
88	A flame-retardant post-synthetically functionalized COF sponge as absorbent for spilled oil recovery. Journal of Materials Science, 2021, 56, 13031.	1.7	6
89	Transport-Relevant Pore Limiting Diameter for Molecular Separations in Metalâ€“Organic Framework Membranes. Journal of Physical Chemistry C, 2021, 125, 20416-20425.	1.5	6
90	Deep learning neural network potential for simulating gaseous adsorption in metalâ€“organic frameworks. Materials Advances, 2022, 3, 5299-5303.	2.6	4

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91	A new measurement of amine steric hindrance â€“ N exposure. Separation and Purification Technology, 2022, 299, 121601.	3.9	4
92	Responses to the comments on â€œMonte Carlo simulations for water adsorption in porous materials: Best practices and new insightsâ€• AICHE Journal, 2022, 68, .	1.8	3
93	In Silico Screening of Zeolites for the Highly Selective Adsorption of Central Câ€“C Bonds toward More Effective Alkane Cracking. Industrial & Engineering Chemistry Research, 2021, 60, 15174-15183.	1.8	2
94	Computational Study of Alkane Adsorption in BrÃ¸nsted Acid Zeolites for More Efficient Alkane Cracking. Langmuir, 2022, 38, 7665-7677.	1.6	2
95	Response to â€œImpact of Zeolite Structure on Entropicâ€“Enthalpic Contributions to Alkane Monomolecular Cracking: An IR Operando Studyâ€• Chemistry - A European Journal, 2019, 25, 7225-7226.	1.7	1
96	InnenrÃ¼cktitelbild: Understanding CO2Dynamics in Metal-Organic Frameworks with Open Metal Sites (Angew. Chem. 16/2013). Angewandte Chemie, 2013, 125, 4589-4589.	1.6	0
97	Understanding BrÃ¸nsted-Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. ChemPhysChem, 2018, 19, 338-338.	1.0	0
98	Frontispiece: Tuning Gas Adsorption by Metal Node Blocking in Photoresponsive Metalâ€“Organic Frameworks. Chemistry - A European Journal, 2018, 24, .	1.7	0