Jianwen Jiang

List of Publications by Year in descending order

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Version: 2024-02-01

279	15,321	12322	24961
papers	citations	69 h-index	109 g-index

285	285	285	14884
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Enhanced Biological Imaging via Aggregation-Induced Emission Active Porous Organic Cages. ACS Nano, 2022, 16, 2355-2368.	7.3	21
2	Machine Learning-Enabled Prediction and High-Throughput Screening of Polymer Membranes for Pervaporation Separation. ACS Applied Materials & Interfaces, 2022, 14, 8427-8436.	4.0	22
3	Free-standing homochiral 2D monolayers by exfoliation of molecular crystals. Nature, 2022, 602, 606-611.	13.7	60
4	Growing single crystals of two-dimensional covalent organic frameworks enabled by intermediate tracing study. Nature Communications, 2022, 13, 1370.	5.8	60
5	Metallated porphyrinic metalâ^'organic frameworks for CO2 conversion to HCOOH: A computational screening and mechanistic study. Molecular Catalysis, 2022, 527, 112407.	1.0	9
6	Recent development in machine learning of polymer membranes for liquid separation. Molecular Systems Design and Engineering, 2022, 7, 856-872.	1.7	7
7	Microscopic insight into anion conduction in covalentâ^'organic framework membranes: A molecular simulation study. Journal of Membrane Science, 2022, , 120754.	4.1	9
8	Accelerating Discovery of High Fractional Free Volume Polymers from a Data-Driven Approach. ACS Applied Materials & Interfaces, 2022, 14, 31203-31215.	4.0	8
9	Confinementâ€Driven Enantioselectivity in 3D Porous Chiral Covalent Organic Frameworks. Angewandte Chemie - International Edition, 2021, 60, 6086-6093.	7.2	48
10	Crystalline Câ€"C and Câ•C Bond-Linked Chiral Covalent Organic Frameworks. Journal of the American Chemical Society, 2021, 143, 369-381.	6.6	117
11	Highly Stable Zr(IV)-Based Metalâ€"Organic Frameworks for Chiral Separation in Reversed-Phase Liquid Chromatography. Journal of the American Chemical Society, 2021, 143, 390-398.	6.6	103
12	Confinementâ€Driven Enantioselectivity in 3D Porous Chiral Covalent Organic Frameworks. Angewandte Chemie, 2021, 133, 6151-6158.	1.6	7
13	In silico screening and design strategies of ethaneâ€selective metalâ€"organic frameworks for ethane/ethylene separation. AICHE Journal, 2021, 67, e17025.	1.8	44
14	Towards complex systems and devices: general discussion. Faraday Discussions, 2021, 225, 431-441.	1.6	0
15	Concluding remarks: Cooperative phenomena in framework materials. Faraday Discussions, 2021, 225, 442-454.	1.6	2
16	Metalâ^'Organic Frameworks for Liquid Phase Applications. Advanced Science, 2021, 8, 2003143.	5.6	21
17	Metalâ€"Organic Frameworks for Xylene Separation: From Computational Screening to Machine Learning. Journal of Physical Chemistry C, 2021, 125, 7839-7848.	1.5	25
18	Highly Selective CO 2 Conversion to Methanol in a Bifunctional Zeolite Catalytic Membrane Reactor. Angewandte Chemie, 2021, 133, 18437-18442.	1.6	1

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19	Highly Selective CO₂ Conversion to Methanol in a Bifunctional Zeolite Catalytic Membrane Reactor. Angewandte Chemie - International Edition, 2021, 60, 18289-18294.	7.2	35
20	Hydrogen Adsorption in Metalâ€“Organic Framework MIL-101(Cr)â€”Adsorbate Densities and Enthalpies from Sorption, Neutron Scattering, In Situ X-ray Diffraction, Calorimetry, and Molecular Simulations. ACS Applied Energy Materials, 2021, 4, 7839-7847.	2.5	2
21	Highly porous nanofiber-supported monolayer graphene membranes for ultrafast organic solvent nanofiltration. Science Advances, 2021, 7, eabg6263.	4.7	75
22	Molecular Simulation Study on Molecularly Mixed Porous Organic Cage/Polymer Composite Membranes for Water Desalination and Solvent Recovery. ACS Applied Nano Materials, 2021, 4, 10378-10388.	2.4	13
23	Materials breaking the rules: general discussion. Faraday Discussions, 2021, 225, 255-270.	1.6	0
24	Novel computational tools: general discussion. Faraday Discussions, 2021, 225, 341-357.	1.6	1
25	Rapid Screening of Metalâ€“Organic Frameworks for Propane/Propylene Separation by Synergizing Molecular Simulation and Machine Learning. ACS Applied Materials & Interfaces, 2021, 13, 53454-53467.	4.0	48
26	Transforming CO₂ into Methanol with N-Heterocyclic Carbene-Stabilized Coinage Metal Hydrides Immobilized in a Metalâ€“Organic Framework UiO-68. ACS Applied Materials & Interfaces, 2021, 13, 58723-58736.	4.0	18
27	Nanostructural Control Enables Optimized Photoacousticâ€“Fluorescenceâ€“Magnetic Resonance Multimodal Imaging and Photothermal Therapy of Brain Tumor. Advanced Functional Materials, 2020, 30, 1907077.	7.8	41
28	Selfâ€Assembly of Highly Stable Zirconium(IV) Coordination Cages with Aggregation Induced Emission Molecular Rotors for Liveâ€Cell Imaging. Angewandte Chemie, 2020, 132, 10237-10245.	1.6	19
29	Selfâ€Assembly of Highly Stable Zirconium(IV) Coordination Cages with Aggregation Induced Emission Molecular Rotors for Liveâ€Cell Imaging. Angewandte Chemie - International Edition, 2020, 59, 10151-10159.	7.2	99
30	Organic Small Molecule Based Photothermal Agents with Molecular Rotors for Malignant Breast Cancer Therapy. Advanced Functional Materials, 2020, 30, 1907093.	7.8	84
31	Porous organic cages as synthetic water channels. Nature Communications, 2020, 11, 4927.	5.8	43
32	Machine Learning for Polymer Swelling in Liquids. ACS Applied Polymer Materials, 2020, 2, 3576-3586.	2.0	19
33	Intercalation of Metal Ions into Ti₃C₂T_x MXene Electrodes for Highâ€Arealâ€Capacitance Microsupercapacitors with Neutral Multivalent Electrolytes. Advanced Functional Materials, 2020, 30, 2003721.	7.8	61
34	Computational design of a metal-based frustrated Lewis pair on defective UiO-66 for CO₂hydrogenation to methanol. Journal of Materials Chemistry A, 2020, 8, 22802-22815.	5.2	27
35	Atomistic Simulation Study of Polyarylate/Zeolitic-Imidazolate Framework Mixed-Matrix Membranes for Water Desalination. ACS Applied Nano Materials, 2020, 3, 10022-10031.	2.4	23
36	All-in-One Molecular Aggregation-Induced Emission Theranostics: Fluorescence Image Guided and Mitochondria Targeted Chemo- and Photodynamic Cancer Cell Ablation. Chemistry of Materials, 2020, 32, 4681-4691.	3.2	73

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37	Dipeptide membranes for CO2 separation: A molecular simulation study. Fluid Phase Equilibria, 2020, 515, 112570.	1.4	5
38	A Highly Rigid and Conjugated Microporous Polymer Membrane for Solvent Permeation and Biofuel Purification: A Molecular Simulation Study. ACS Sustainable Chemistry and Engineering, 2020, 8, 2892-2900.	3.2	14
39	POC/PIM-1 mixed-matrix membranes for water desalination: A molecular simulation study. Journal of Membrane Science, 2020, 608, 118173.	4.1	22
40	Water Permeation through Conical Nanopores: Complex Interplay between Surface Roughness and Chemistry. Advanced Theory and Simulations, 2020, 3, 2000025.	1.3	6
41	Molecular simulations of liquid separations in polymer membranes. Current Opinion in Chemical Engineering, 2020, 28, 66-74.	3.8	22
42	Functional UiO-66 for the removal of sulfur-containing compounds in gas and liquid mixtures: A molecular simulation study. Chemical Engineering Journal, 2019, 356, 737-745.	6.6	15
43	Effects of functionalization on the nanofiltration performance of PIM-1: Molecular simulation investigation. Journal of Membrane Science, 2019, 591, 117357.	4.1	17
44	Chiral Phosphoric Acids in Metalâ€“Organic Frameworks with Enhanced Acidity and Tunable Catalytic Selectivity. Angewandte Chemie - International Edition, 2019, 58, 14748-14757.	7.2	50
45	Boosting Enantioselectivity of Chiral Organocatalysts with Ultrathin Two-Dimensional Metalâ€“Organic Framework Nanosheets. Journal of the American Chemical Society, 2019, 141, 17685-17695.	6.6	128
46	Formation of CH₄ Hydrate in a Mesoporous Metalâ€“Organic Framework MIL-101: Mechanistic Insights from Microsecond Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2019, 10, 7002-7008.	2.1	35
47	Microporous benzimidazole-linked polymer and its derivatives for organic solvent nanofiltration. Polymer, 2019, 185, 121932.	1.8	10
48	Chiral Phosphoric Acids in Metalâ€“Organic Frameworks with Enhanced Acidity and Tunable Catalytic Selectivity. Angewandte Chemie, 2019, 131, 14890-14899.	1.6	16
49	Post-synthesis of a covalent organic framework nanofiltration membrane for highly efficient water treatment. Journal of Materials Chemistry A, 2019, 7, 24205-24210.	5.2	101
50	Molecular design of chiral zirconium metalâ€“organic frameworks for asymmetric transfer hydrogenation of imines. Catalysis Science and Technology, 2019, 9, 4888-4897.	2.1	9
51	A molecular simulation study for efficient separation of 2,5-furandiyldimethanamine by a microporous polyarylate membrane. Polymer, 2019, 175, 8-14.	1.8	7
52	Enhancing water permeation through alumina membranes by changing from cylindrical to conical nanopores. Nanoscale, 2019, 11, 9869-9878.	2.8	25
53	Identifying the best metalâ€“organic frameworks and unravelling different mechanisms for the separation of pentane isomers. Molecular Systems Design and Engineering, 2019, 4, 609-615.	1.7	8
54	Chiral BINOL-Based Covalent Organic Frameworks for Enantioselective Sensing. Journal of the American Chemical Society, 2019, 141, 7081-7089.	6.6	245

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55	Computational screening of metalâ"organic frameworks for CO2 separation. Current Opinion in Green and Sustainable Chemistry, 2019, 16, 57-64.	3.2	15
56	Molecular Design of Microporous Polymer Membranes for the Upgrading of Natural Gas. Journal of Physical Chemistry C, 2019, 123, 6607-6615.	1.5	17
57	A molecular simulation protocol for swelling and organic solvent nanofiltration of polymer membranes. Journal of Membrane Science, 2019, 573, 639-646.	4.1	50
58	Computational Design of 2D Covalent-Organic Framework Membranes for Organic Solvent Nanofiltration. ACS Sustainable Chemistry and Engineering, 2019, 7, 1734-1744.	3.2	52
59	A molecular simulation protocol for membrane pervaporation. Journal of Membrane Science, 2019, 572, 676-682.	4.1	22
60	Hydrophobic Shielding of Outer Surface: Enhancing the Chemical Stability of Metalâ€"Organic Polyhedra. Angewandte Chemie, 2019, 131, 1053-1057.	1.6	8
61	Restriction of Molecular Rotors in Ultrathin Two-Dimensional Covalent Organic Framework Nanosheets for Sensing Signal Amplification. Chemistry of Materials, 2019, 31, 146-160.	3.2	125
62	Hydrophobic Shielding of Outer Surface: Enhancing the Chemical Stability of Metalâ€"Organic Polyhedra. Angewandte Chemie - International Edition, 2019, 58, 1041-1045.	7.2	45
63	CO2 cycloaddition with propylene oxide to form propylene carbonate on a copper metal-organic framework: A density functional theory study. Molecular Catalysis, 2019, 463, 37-44.	1.0	28
64	Porous organic cages embedded in a lipid membrane for water desalination: A molecular simulation study. Journal of Membrane Science, 2019, 573, 177-183.	4.1	24
65	Methanol-to-olefin conversion in ABC-6 zeolite cavities: unravelling the role of cavity shape and size from density functional theory calculations. Physical Chemistry Chemical Physics, 2018, 20, 14322-14330.	1.3	8
66	Confinement of Aggregation-Induced Emission Molecular Rotors in Ultrathin Two-Dimensional Porous Organic Nanosheets for Enhanced Molecular Recognition. Journal of the American Chemical Society, 2018, 140, 4035-4046.	6.6	119
67	Dipeptide Crystals as Reverse Osmosis Membranes for Water Desalination: Atomistic Simulation. Journal of Physical Chemistry C, 2018, 122, 6026-6032.	1.5	13
68	Efficient Removal of Pb²⁺ from Aqueous Solution by an Ionic Covalentâ€"Organic Framework: Molecular Simulation Study. Industrial & Engineering Chemistry Research, 2018, 57, 6477-6482.	1.8	33
69	High-throughput computational screening of metal-organic framework membranes for upgrading of natural gas. Journal of Membrane Science, 2018, 551, 47-54.	4.1	73
70	Amorphous Porous Organic Cage Membranes for Water Desalination. Journal of Physical Chemistry C, 2018, 122, 1732-1740.	1.5	25
71	Catalytic amino acid production from biomass-derived intermediates. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 5093-5098.	3.3	168
72	Water desalination and biofuel dehydration through a thin membrane of polymer of intrinsic microporosity: Atomistic simulation study. Journal of Membrane Science, 2018, 545, 49-56.	4.1	55

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73	Frontispiece: Highâ€Flux Highâ€Selectivity Metalâ€“Organic Framework MILâ€160 Membrane for Xylene Isomer Separation by Pervaporation. Angewandte Chemie - International Edition, 2018, 57, .	7.2	0
74	Hochflussâ€HochselektivitÃtsâ€MOFâ€Membran: GetrÃgerte MILâ€160â€Schicht fÃ¼r die Trennung der Xylolisomere durch Pervaporation. Angewandte Chemie, 2018, 130, 15580-15584.	1.6	14
75	Frontispiz: Hochflussâ€HochselektivitÃtsâ€MOFâ€Membran: GetrÃgerte MILâ€160â€Schicht fÃ¼r die Trennung der Xylolisomere durch Pervaporation. Angewandte Chemie, 2018, 130, .	1.6	0
76	Molecular Simulation and Analysis of Sorption Process toward Theoretical Prediction for Liquid Permeation through Membranes. Journal of Physical Chemistry B, 2018, 122, 12211-12218.	1.2	7
77	Highâ€Flux Highâ€Selectivity Metalâ€“Organic Framework MILâ€160 Membrane for Xylene Isomer Separation by Pervaporation. Angewandte Chemie - International Edition, 2018, 57, 15354-15358.	7.2	101
78	Design and self-assembly of hexahedral coordination cages for cascade reactions. Nature Communications, 2018, 9, 4423.	5.8	85
79	Zeolitic Imidazolate Framework Membranes for Organic Solvent Nanofiltration: A Molecular Simulation Exploration. ACS Applied Materials & Interfaces, 2018, 10, 33135-33143.	4.0	26
80	Computational Characterization of Ultrathin Polymer Membranes in Liquids. Macromolecules, 2018, 51, 7169-7177.	2.2	37
81	Computational screening of hydrophobic metalâ€“organic frameworks for the separation of H₂S and CO₂ from natural gas. Journal of Materials Chemistry A, 2018, 6, 18898-18905.	5.2	84
82	Solvent nanofiltration through polybenzimidazole membranes: Unravelling the role of pore size from molecular simulations. Journal of Membrane Science, 2018, 564, 782-787.	4.1	18
83	Decomposition of CH₄ hydrate: effects of temperature and salt from molecular simulations. Molecular Simulation, 2018, 44, 1220-1228.	0.9	18
84	Chiral NH-Controlled Supramolecular Metallacycles. Journal of the American Chemical Society, 2017, 139, 1554-1564.	6.6	122
85	Reversed thermo-switchable molecular sieving membranes composed of two-dimensional metal-organic nanosheets for gas separation. Nature Communications, 2017, 8, 14460.	5.8	382
86	Water Desalination through a Zeolitic Imidazolate Framework Membrane by Electro- and Thermo-Osmosis: Which Could Be More Efficient?. ChemistrySelect, 2017, 2, 3981-3986.	0.7	5
87	What are the key factors governing the nucleation of CO₂ hydrate?. Physical Chemistry Chemical Physics, 2017, 19, 15657-15661.	1.3	75
88	Computational design of 2D functional covalentâ€“organic framework membranes for water desalination. Environmental Science: Water Research and Technology, 2017, 3, 735-743.	1.2	69
89	Porous organic cage membranes for water desalination: a simulation exploration. Physical Chemistry Chemical Physics, 2017, 19, 18178-18185.	1.3	25
90	Molecular Design of Zirconium Tetrazolate Metalâ€“Organic Frameworks for CO₂ Capture. Crystal Growth and Design, 2017, 17, 543-549.	1.4	36

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91	1D-2D-3D Transformation Synthesis of Hierarchical Metalâ€“Organic Framework Adsorbent for Multicomponent Alkane Separation. Journal of the American Chemical Society, 2017, 139, 819-828.	6.6	62
92	Ultrathin two-dimensional porous organic nanosheets with molecular rotors for chemical sensing. Nature Communications, 2017, 8, 1142.	5.8	152
93	CH₄ Hydrate Formation between Silica and Graphite Surfaces: Insights from Microsecond Molecular Dynamics Simulations. Langmuir, 2017, 33, 11956-11967.	1.6	80
94	High-Throughput Computational Screening of Metalâ€“Organic Frameworks for Thiol Capture. Journal of Physical Chemistry C, 2017, 121, 22208-22215.	1.5	38
95	Ethanolamine Purification by Nanofiltration through PIM-1 and Carbon Membranes: A Molecular Simulation Study. Journal of Physical Chemistry C, 2017, 121, 20539-20545.	1.5	11
96	Dipeptides Embedded in a Lipid Bilayer Membrane as Synthetic Water Channels. Langmuir, 2017, 33, 11490-11495.	1.6	4
97	Molecular Dynamics Phenomena of Water in the Metalorganic Framework MIL-100(Al), as Revealed by Pulsed Field Gradient NMR and Atomistic Simulation. Journal of Physical Chemistry C, 2017, 121, 18065-18074.	1.5	25
98	Seawater Pervaporation through Zeolitic Imidazolate Framework Membranes: Atomistic Simulation Study. ACS Applied Materials & Interfaces, 2016, 8, 13392-13399.	4.0	72
99	High-throughput computational screening of 137953 metalâ€“organic frameworks for membrane separation of a CO₂/N₂/CH₄ mixture. Journal of Materials Chemistry A, 2016, 4, 15904-15912.	5.2	99
100	pH-Sensitive Vesicles Formed by Amphiphilic Grafted Copolymers with Tunable Membrane Permeability for Drug Loading/Release: A Multiscale Simulation Study. Macromolecules, 2016, 49, 6084-6094.	2.2	58
101	Molecular Insights into the Nucleation and Growth of CH₄ and CO₂ Mixed Hydrates from Microsecond Simulations. Journal of Physical Chemistry C, 2016, 120, 25225-25236.	1.5	84
102	A helical peptide confined in metal-organic frameworks: Microscopic insight from molecular simulation. Microporous and Mesoporous Materials, 2016, 232, 138-142.	2.2	7
103	Modulated Hydrothermal Synthesis of UiO-66(Hf)-Type Metalâ€“Organic Frameworks for Optimal Carbon Dioxide Separation. Inorganic Chemistry, 2016, 55, 1134-1141.	1.9	161
104	Synthesis and seawater desalination of molecular sieving zeolitic imidazolate framework membranes. Desalination, 2016, 385, 75-82.	4.0	137
105	In silico screening of 4764 computation-ready, experimental metalâ€“organic frameworks for CO₂ separation. Journal of Materials Chemistry A, 2016, 4, 2105-2114.	5.2	109
106	Design of amine-functionalized metalâ€“organic frameworks for CO₂ separation: the more amine, the better?. Chemical Communications, 2016, 52, 974-977.	2.2	76
107	Ibuprofen loading and release in amphiphilic peptide FA32 and its derivatives: a coarse-grained molecular dynamics simulation study. Molecular Simulation, 2016, 42, 679-687.	0.9	9
108	Porous Materials: Submicrometer-Sized ZIF-71 Filled Organophilic Membranes for Improved Bioethanol Recovery: Mechanistic Insights by Monte Carlo Simulation and FTIR Spectroscopy (Adv. Funct. Mater.) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	7.8	1

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109	Glucose recovery from aqueous solutions by adsorption in metalâ€“organic framework MIL-101: a molecular simulation study. Scientific Reports, 2015, 5, 12821.	1.6	11
110	Biofuel purification in GME zeoliticâ€“imidazolate frameworks: From ab initio calculations to molecular simulations. AICHE Journal, 2015, 61, 2763-2775.	1.8	22
111	Computational Amphiphilic Materials for Drug Delivery. Frontiers in Materials, 2015, 2, .	1.2	24
112	Submicrometerâ€Sized ZIFâ€71 Filled Organophilic Membranes for Improved Bioethanol Recovery: Mechanistic Insights by Monte Carlo Simulation and FTIR Spectroscopy. Advanced Functional Materials, 2015, 25, 516-525.	7.8	94
113	CO₂ capture in rht metalâ€“organic frameworks: multiscale modeling from molecular simulation to breakthrough prediction. Journal of Materials Chemistry A, 2015, 3, 16327-16336.	5.2	20
114	Water Desalination through Zeolitic Imidazolate Framework Membranes: Significant Role of Functional Groups. Langmuir, 2015, 31, 13230-13237.	1.6	108
115	Cellulose dissolution and regeneration in ionic liquids: A computational perspective. Chemical Engineering Science, 2015, 121, 180-189.	1.9	111
116	CO2 capture in cation-exchanged metalâ€“organic frameworks: Holistic modeling from molecular simulation to process optimization. Chemical Engineering Science, 2015, 124, 70-78.	1.9	44
117	Molecular insights into the self-assembly of short amphiphilic peptides FmDn and FmKn. RSC Advances, 2014, 4, 60741-60748.	1.7	9
118	Mechanistic insight into highly efficient gas permeation and separation in a shape-persistent ladder polymer membrane. Physical Chemistry Chemical Physics, 2014, 16, 6075.	1.3	49
119	Synthesis of highly hydrophobic and permselective metalâ€“organic framework Zn(BDC)(TED)0.5 membranes for H2/CO2 separation. Journal of Membrane Science, 2014, 454, 126-132.	4.1	55
120	Enhancement of CO₂uptake in iso-reticular Co based zeolitic imidazolate frameworks via metal replacement. CrystEngComm, 2014, 16, 4677-4680.	1.3	32
121	Covalent-organic framework as a template to assemble carbon nanotubes into a high-density membrane: computational demonstration. Nanoscale, 2014, 6, 772-777.	2.8	4
122	Molecular simulations in metalâ€“organic frameworks for diverse potential applications. Molecular Simulation, 2014, 40, 516-536.	0.9	31
123	Self-Assembly of Amphiphilic Peptide (AF)6H5K15 Derivatives: Roles of Hydrophilic and Hydrophobic Residues. Journal of Physical Chemistry B, 2014, 118, 2683-2692.	1.2	21
124	A Combinatorial Approach towards Waterâ€Stable Metalâ€“Organic Frameworks for Highly Efficient Carbon Dioxide Separation. ChemSusChem, 2014, 7, 2791-2795.	3.6	82
125	Adsorption and Diffusion of CO₂ and CH₄ in Zeolitic Imidazolate Framework-8: Effect of Structural Flexibility. Journal of Physical Chemistry C, 2014, 118, 8788-8794.	1.5	132
126	â€œClickâ€•extended nitrogen-rich metalâ€“organic frameworks and their high performance in CO2-selective capture. Chemical Communications, 2014, 50, 4683.	2.2	61

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127	Systematic Investigation of Nitrile Based Ionic Liquids for CO₂ Capture: A Combination of Molecular Simulation and ab Initio Calculation. Journal of Physical Chemistry C, 2014, 118, 3110-3118.	1.5	44
128	Engineering chiral porous metal-organic frameworks for enantioselective adsorption and separation. Nature Communications, 2014, 5, 4406.	5.8	221
129	Biofuel purification in zeolitic imidazolate frameworks: the significant role of functional groups. Physical Chemistry Chemical Physics, 2014, 16, 9643-9655.	1.3	57
130	Crucial role of blocking inaccessible cages in the simulation of gas adsorption in a paddle-wheel metalâ€“organic framework. RSC Advances, 2013, 3, 16152.	1.7	15
131	Self-Assembly of Amphiphilic Peptide (AF)₆H₅K₁₅: Coarse-Grained Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2013, 117, 9690-9698.	1.2	39
132	Adsorption of C₁â€“C₄ Alcohols in Zeolitic Imidazolate Framework-8: Effects of Force Fields, Atomic Charges, and Framework Flexibility. Journal of Physical Chemistry C, 2013, 117, 25628-25635.	1.5	70
133	Ag nanoprisms with Ag2S attachment. Scientific Reports, 2013, 3, 2177.	1.6	61
134	Engineering nanostructured materials for sustainable future. Asia-Pacific Journal of Chemical Engineering, 2013, 8, 203-204.	0.8	0
135	Thermal Conductivity of Zeolitic Imidazolate Framework-8: A Molecular Simulation Study. Journal of Physical Chemistry C, 2013, 117, 18441-18447.	1.5	117
136	Ionic Liquid Membranes Supported by Hydrophobic and Hydrophilic Metalâ€“Organic Frameworks for CO₂ Capture. Journal of Physical Chemistry C, 2013, 117, 5792-5799.	1.5	79
137	Functionalized metalâ€“organic framework MIL-101 for CO2 capture: multi-scale modeling from ab initio calculation and molecular simulation to breakthrough prediction. CrystEngComm, 2013, 15, 10358.	1.3	36
138	Cellulose regeneration from a cellulose/ionic liquid mixture: the role of anti-solvents. RSC Advances, 2013, 3, 12794.	1.7	68
139	CO₂capture in poly(ionic liquid) membranes: atomistic insight into the role of anions. Physical Chemistry Chemical Physics, 2013, 15, 651-658.	1.3	55
140	Liquid Chromatographic Separation in Metalâ€“Organic Framework MIL-101: A Molecular Simulation Study. Langmuir, 2013, 29, 1650-1656.	1.6	17
141	Sorption-Induced Structural Transition of Zeolitic Imidazolate Framework-8: A Hybrid Molecular Simulation Study. Journal of the American Chemical Society, 2013, 135, 3722-3728.	6.6	160
142	A Rationally Designed Nitrogen-Rich Metal-Organic Framework and Its Exceptionally High CO2 and H2 Uptake Capability. Scientific Reports, 2013, 3, 1149.	1.6	122
143	Propylene/Propane Separation Using SiCHA. Industrial & Engineering Chemistry Research, 2013, 52, 3877-3892.	1.8	41
144	Atomistic insight into micro-phase separation and gas diffusion in PEOâ€“PBT multiblock copolymers. Molecular Simulation, 2013, 39, 902-907.	0.9	4

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145	Molecular insight into cellulose regeneration from a cellulose/ionic liquid mixture: effects of water concentration and temperature. RSC Advances, 2013, 3, 4425.	1.7	48
146	Self-Templated Free-Radical Polymerization To Form Tactic Chains in Confined Environment. Journal of Physical Chemistry B, 2013, 117, 7826-7832.	1.2	1
147	Bovine pancreatic trypsin inhibitor crystals with different morphologies: a molecular dynamics simulation study. Molecular Simulation, 2012, 38, 112-118.	0.9	1
148	CO₂ Adsorption in Mono-, Di- and Trivalent Cation-Exchanged Metalâ€“Organic Frameworks: A Molecular Simulation Study. Langmuir, 2012, 28, 3903-3910.	1.6	39
149	Development of a force field for zeolitic imidazolate framework-8 with structural flexibility. Journal of Chemical Physics, 2012, 136, 244703.	1.2	67
150	A homochiral metalâ€“organic framework membrane for enantioselective separation. Chemical Communications, 2012, 48, 7022.	2.2	139
151	Ion Exchange in Metalâ€“Organic Framework for Water Purification: Insight from Molecular Simulation. Journal of Physical Chemistry C, 2012, 116, 6925-6931.	1.5	77
152	Metalâ€“Organic Framework/Polymer Mixed-Matrix Membranes for H₂/CO₂ Separation: A Fully Atomistic Simulation Study. Journal of Physical Chemistry C, 2012, 116, 19268-19277.	1.5	72
153	Crowding effect on DNA melting: a molecular thermodynamic model with explicit solvent. Physical Chemistry Chemical Physics, 2012, 14, 15400.	1.3	10
154	Recent development of in silico molecular modeling for gas and liquid separations in metalâ€“organic frameworks. Current Opinion in Chemical Engineering, 2012, 1, 138-144.	3.8	19
155	Recovery of Dimethyl Sulfoxide from Aqueous Solutions by Highly Selective Adsorption in Hydrophobic Metalâ€“Organic Frameworks. Langmuir, 2012, 28, 15305-15312.	1.6	22
156	A highly permeable and selective zeolitic imidazolate framework ZIF-95 membrane for H2/CO2 separation. Chemical Communications, 2012, 48, 10981.	2.2	197
157	Metalâ€“organic framework supported ionic liquid membranes for CO2 capture: anion effects. Physical Chemistry Chemical Physics, 2012, 14, 5785.	1.3	113
158	Dendritic Ptâ€“Cu bimetallic nanocrystals with a high electrocatalytic activity toward methanol oxidation. Materials Chemistry and Physics, 2012, 132, 244-247.	2.0	37
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