Jianwen Jiang

List of Publications by Year in descending order

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279 papers	15,321 citations	12330 69 h-index	24982 109 g-index
285 all docs	285 docs citations	285 times ranked	14884 citing authors

#	Article	IF	Citations
1	A high-performance asymmetric supercapacitor fabricated with graphene-based electrodes. Energy and Environmental Science, 2011, 4, 4009.	30.8	741
2	Storage and Separation of CO2and CH4in Silicalite, C168Schwarzite, and IRMOF-1:Â A Comparative Study from Monte Carlo Simulation. Langmuir, 2007, 23, 659-666.	3.5	388
3	Reversed thermo-switchable molecular sieving membranes composed of two-dimensional metal-organic nanosheets for gas separation. Nature Communications, 2017, 8, 14460.	12.8	382
4	Synthesis and Capacitive Properties of Manganese Oxide Nanosheets Dispersed on Functionalized Graphene Sheets. Journal of Physical Chemistry C, 2011, 115, 6448-6454.	3.1	365
5	Chiral BINOL-Based Covalent Organic Frameworks for Enantioselective Sensing. Journal of the American Chemical Society, 2019, 141, 7081-7089.	13.7	245
6	Molecular Screening of Metalâ"Organic Frameworks for CO₂ Storage. Langmuir, 2008, 24, 6270-6278.	3.5	227
7	Engineering chiral porous metal-organic frameworks for enantioselective adsorption and separation. Nature Communications, 2014, 5, 4406.	12.8	221
8	Amino functionalized zeolitic tetrazolate framework (ZTF) with high capacity for storage of carbon dioxide. Chemical Communications, 2011, 47, 2011-2013.	4.1	218
9	Unprecedentedly High Selective Adsorption of Gas Mixtures in rho Zeolite-like Metalâ"Organic Framework: A Molecular Simulation Study. Journal of the American Chemical Society, 2009, 131, 11417-11425.	13.7	202
10	A highly permeable and selective zeolitic imidazolate framework ZIF-95 membrane for H2/CO2 separation. Chemical Communications, 2012, 48, 10981.	4.1	197
11	Zeolitic imidazolate framework-8 as a reverse osmosis membrane for water desalination: Insight from molecular simulation. Journal of Chemical Physics, 2011, 134, 134705.	3.0	182
12	Molecular dynamics and dissipative particle dynamics simulations for the miscibility of poly(ethylene) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	3.8	171
13	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.	7.1	168
14	Modulated Hydrothermal Synthesis of UiO-66(Hf)-Type Metalâ€"Organic Frameworks for Optimal Carbon Dioxide Separation. Inorganic Chemistry, 2016, 55, 1134-1141.	4.0	161
15	Sorption-Induced Structural Transition of Zeolitic Imidazolate Framework-8: A Hybrid Molecular Simulation Study. Journal of the American Chemical Society, 2013, 135, 3722-3728.	13.7	160
16	pH-sensitive drug loading/releasing in amphiphilic copolymer PAEâ€"PEG: Integrating molecular dynamics and dissipative particle dynamics simulations. Journal of Controlled Release, 2012, 162, 185-193.	9.9	157
17	Ultrathin two-dimensional porous organic nanosheets with molecular rotors for chemical sensing. Nature Communications, 2017, 8, 1142.	12.8	152
18	Template Synthesis of Tubular Ruthenium Oxides for Supercapacitor Applications. Journal of Physical Chemistry C, 2010, 114, 13608-13613.	3.1	144

#	Article	IF	Citations
19	Diffusion and Separation of CO₂ and CH₄ in Silicalite, C₁₆₈ Schwarzite, and IRMOF-1: A Comparative Study from Molecular Dynamics Simulation. Langmuir, 2008, 24, 5474-5484.	3.5	140
20	A homochiral metalâ€“organic framework membrane for enantioselective separation. Chemical Communications, 2012, 48, 7022.	4.1	139
21	Synthesis and seawater desalination of molecular sieving zeolitic imidazolate framework membranes. Desalination, 2016, 385, 75-82.	8.2	137
22	Molecular Simulations for Adsorptive Separation of CO₂/CH₄ Mixture in Metal-Exposed, Catenated, and Charged Metalâ^'Organic Frameworks. Langmuir, 2009, 25, 5239-5247.	3.5	134
23	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.	3.1	132
24	Molecular simulations for energy, environmental and pharmaceutical applications of nanoporous materials: from zeolites, metalâ€“organic frameworks to protein crystals. Chemical Society Reviews, 2011, 40, 3599.	38.1	130
25	Boosting Enantioselectivity of Chiral Organocatalysts with Ultrathin Two-Dimensional Metalâ€“Organic Framework Nanosheets. Journal of the American Chemical Society, 2019, 141, 17685-17695.	13.7	128
26	Exceptionally high CO2 storage in covalent-organic frameworks: Atomistic simulation study. Energy and Environmental Science, 2008, 1, 139.	30.8	126
27	Restriction of Molecular Rotors in Ultrathin Two-Dimensional Covalent Organic Framework Nanosheets for Sensing Signal Amplification. Chemistry of Materials, 2019, 31, 146-160.	6.7	125
28	A Rationally Designed Nitrogen-Rich Metal-Organic Framework and Its Exceptionally High CO2 and H2 Uptake Capability. Scientific Reports, 2013, 3, 1149.	3.3	122
29	Chiral NH-Controlled Supramolecular Metallacycles. Journal of the American Chemical Society, 2017, 139, 1554-1564.	13.7	122
30	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.	13.7	119
31	Monte Carlo Simulation for the Adsorption and Separation of Linear and Branched Alkanes in IRMOF-1. Langmuir, 2006, 22, 5702-5707.	3.5	118
32	Thermal Conductivity of Zeolitic Imidazolate Framework-8: A Molecular Simulation Study. Journal of Physical Chemistry C, 2013, 117, 18441-18447.	3.1	117
33	Crystalline Câ€”C and Câ•C Bond-Linked Chiral Covalent Organic Frameworks. Journal of the American Chemical Society, 2021, 143, 369-381.	13.7	117
34	Ionic Liquid/Metalâ€“Organic Framework Composite for CO₂ Capture: A Computational Investigation. Journal of Physical Chemistry C, 2011, 115, 21736-21742.	3.1	114
35	Metalâ^'Organic Framework MIL-101 for Adsorption and Effect of Terminal Water Molecules: From Quantum Mechanics to Molecular Simulation. Langmuir, 2010, 26, 8743-8750.	3.5	113
36	Metalâ€“organic framework supported ionic liquid membranes for CO2 capture: anion effects. Physical Chemistry Chemical Physics, 2012, 14, 5785.	2.8	113

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37	Molecular Understanding for the Adsorption of Water and Alcohols in Hydrophilic and Hydrophobic Zeolitic Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2010, 114, 11542-11550.	3.1	111
38	Cellulose dissolution and regeneration in ionic liquids: A computational perspective. Chemical Engineering Science, 2015, 121, 180-189.	3.8	111
39	In silico screening of 4764 computation-ready, experimental metalâ€"organic frameworks for CO₂ separation. Journal of Materials Chemistry A, 2016, 4, 2105-2114.	10.3	109
40	Water Desalination through Zeolitic Imidazolate Framework Membranes: Significant Role of Functional Groups. Langmuir, 2015, 31, 13230-13237.	3.5	108
41	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.	13.7	103
42	Fluorinated Metalâ€"Organic Frameworks: Advantageous for Higher H₂ and CO₂ Adsorption or Not?. Chemistry - A European Journal, 2012, 18, 688-694.	3.3	101
43	Highâ€Flux Highâ€Selectivity Metalâ€"Organic Framework MILâ€160 Membrane for Xylene Isomer Separation by Pervaporation. Angewandte Chemie - International Edition, 2018, 57, 15354-15358.	13.8	101
44	Post-synthesis of a covalent organic framework nanofiltration membrane for highly efficient water treatment. Journal of Materials Chemistry A, 2019, 7, 24205-24210.	10.3	101
45	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.	10.3	99
46	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.	13.8	99
47	Unraveling the Energetics and Dynamics of Ibuprofen in Mesoporous Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2009, 113, 18287-18291.	3.1	97
48	A Bioâ€Metalâ€"Organic Framework for Highly Selective CO₂ Capture: A Molecular Simulation Study. ChemSusChem, 2010, 3, 982-988.	6.8	95
49	A Highly Hydrophobic Metalâ^'Organic Framework Zn(BDC)(TED)0.5 for Adsorption and Separation of CH3OH/H2O and CO2/CH4: An Integrated Experimental and Simulation Study. Journal of Physical Chemistry C, 2010, 114, 6602-6609.	3.1	94
50	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.	14.9	94
51	Equation of state for thermodynamic properties of chain fluids near-to and far-from the vaporâ€"liquid critical region. Journal of Chemical Physics, 1999, 111, 5964-5974.	3.0	93
52	Adsorption and separation of linear and branched alkanes on carbon nanotube bundles from configurational-bias Monte Carlo simulation. Physical Review B, 2005, 72, .	3.2	93
53	Design and self-assembly of hexahedral coordination cages for cascade reactions. Nature Communications, 2018, 9, 4423.	12.8	85
54	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.	3.1	84

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55	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.	10.3	84
56	Organic Small Molecule Based Photothermal Agents with Molecular Rotors for Malignant Breast Cancer Therapy. Advanced Functional Materials, 2020, 30, 1907093.	14.9	84
57	A Combinatorial Approach towards Waterâ€Stable Metalâ€“Organic Frameworks for Highly Efficient Carbon Dioxide Separation. ChemSusChem, 2014, 7, 2791-2795.	6.8	82
58	CH₄ Hydrate Formation between Silica and Graphite Surfaces: Insights from Microsecond Molecular Dynamics Simulations. Langmuir, 2017, 33, 11956-11967.	3.5	80
59	Effects of Solvent Viscosity on Protein Dynamics:â€‰ Infrared Vibrational Echo Experiments and Theory. Journal of Physical Chemistry B, 2001, 105, 1081-1092.	2.6	79
60	Structural Isomerism and Effect of Fluorination on Gas Adsorption in Copper-Tetrazolate Based Metal Organic Frameworks. Chemistry of Materials, 2011, 23, 2908-2916.	6.7	79
61	Ionic Liquid Membranes Supported by Hydrophobic and Hydrophilic Metalâ€“Organic Frameworks for CO₂ Capture. Journal of Physical Chemistry C, 2013, 117, 5792-5799.	3.1	79
62	Ion Exchange in Metalâ€“Organic Framework for Water Purification: Insight from Molecular Simulation. Journal of Physical Chemistry C, 2012, 116, 6925-6931.	3.1	77
63	Separation of CO2 and N2 by Adsorption in C168 Schwarzite:â€‰ A Combination of Quantum Mechanics and Molecular Simulation Study. Journal of the American Chemical Society, 2005, 127, 11989-11997.	13.7	76
64	Design of amine-functionalized metalâ€“organic frameworks for CO₂ separation: the more amine, the better?. Chemical Communications, 2016, 52, 974-977.	4.1	76
65	What are the key factors governing the nucleation of CO₂ hydrate?. Physical Chemistry Chemical Physics, 2017, 19, 15657-15661.	2.8	75
66	Highly porous nanofiber-supported monolayer graphene membranes for ultrafast organic solvent nanofiltration. Science Advances, 2021, 7, eabg6263.	10.3	75
67	High-throughput computational screening of metal-organic framework membranes for upgrading of natural gas. Journal of Membrane Science, 2018, 551, 47-54.	8.2	73
68	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.	6.7	73
69	A molecular-thermodynamic model for polyelectrolyte solutions. Journal of Chemical Physics, 1998, 108, 780-784.	3.0	72
70	Highly Porous Ionic rht Metalâ”Organic Framework for H2 and CO2 Storage and Separation: A Molecular Simulation Study. Langmuir, 2010, 26, 11196-11203.	3.5	72
71	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.	3.1	72
72	Seawater Pervaporation through Zeolitic Imidazolate Framework Membranes: Atomistic Simulation Study. ACS Applied Materials & Interfaces, 2016, 8, 13392-13399.	8.0	72

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73	Capillary Phase Transitions ofn-Alkanes in a Carbon Nanotube. Nano Letters, 2004, 4, 241-244.	9.1	71
74	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.	3.1	70
75	Computational design of 2D functional covalentâ€“organic framework membranes for water desalination. Environmental Science: Water Research and Technology, 2017, 3, 735-743.	2.4	69
76	Cellulose regeneration from a cellulose/ionic liquid mixture: the role of anti-solvents. RSC Advances, 2013, 3, 12794.	3.6	68
77	Upgrade of natural gas in rho zeolite-like metalâ€“organic framework and effect of water: a computational study. Energy and Environmental Science, 2009, 2, 1088.	30.8	67
78	Mechanistic understanding of CO2-induced plasticization of a polyimide membrane: A combination of experiment and simulation study. Polymer, 2010, 51, 4439-4447.	3.8	67
79	Development of a force field for zeolitic imidazolate framework-8 with structural flexibility. Journal of Chemical Physics, 2012, 136, 244703.	3.0	67
80	Thermodynamic properties and phase equilibria of charged hard sphere chain model for polyelectrolyte solutions. Molecular Physics, 2001, 99, 1121-1128.	1.7	66
81	Density Functional Theory for Adsorption of Gas Mixtures in Metalâ^'Organic Frameworks. Journal of Physical Chemistry B, 2010, 114, 2820-2827.	2.6	65
82	Interactions between bovine serum albumin and gemini surfactant alkanediyl-Î±, Ï‰-bis(dimethyldodecyl-ammonium bromide). Biopolymers, 2006, 83, 243-249.	2.4	63
83	Nitrogen adsorption on carbon nanotube bundles:â€‚â€‚Role of the external surface. Physical Review B, 2003, 68, .	3.2	62
84	Nitrogen and Oxygen Mixture Adsorption on Carbon Nanotube Bundles from Molecular Simulation. Langmuir, 2004, 20, 10910-10918.	3.5	62
85	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.	13.7	62
86	Gas Permeation and Separation in Functionalized Polymers of Intrinsic Microporosity: A Combination of Molecular Simulations and Ab Initio Calculations. Journal of Physical Chemistry C, 2011, 115, 14123-14130.	3.1	61
87	Ag nanoprisms with Ag2S attachment. Scientific Reports, 2013, 3, 2177.	3.3	61
88	â€œClickâ€•extended nitrogen-rich metalâ€“organic frameworks and their high performance in CO2-selective capture. Chemical Communications, 2014, 50, 4683.	4.1	61
89	Intercalation of Metal Ions into Ti₃C₂T_x MXene Electrodes for Highâ€Arealâ€Capacitance Microsupercapacitors with Neutral Multivalent Electrolytes. Advanced Functional Materials, 2020, 30, 2003721.	14.9	61
90	Free-standing homochiral 2D monolayers by exfoliation of molecular crystals. Nature, 2022, 602, 606-611.	27.8	60

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91	Growing single crystals of two-dimensional covalent organic frameworks enabled by intermediate tracing study. Nature Communications, 2022, 13, 1370.	12.8	60
92	A New Model for the Viscosity of Electrolyte Solutions. Industrial & Engineering Chemistry Research, 2003, 42, 6267-6272.	3.7	58
93	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.	4.8	58
94	Biofuel purification in zeolitic imidazolate frameworks: the significant role of functional groups. Physical Chemistry Chemical Physics, 2014, 16, 9643-9655.	2.8	57
95	Computer Simulation for Adsorption of CO₂, N₂and Flue Gas in a Mimetic MCM-41. Journal of Physical Chemistry C, 2008, 112, 11295-11300.	3.1	55
96	Charged soc metalâ€organic framework for highâ€efficacy H₂ adsorption and syngas purification: Atomistic simulation study. AIChE Journal, 2009, 55, 2422-2432.	3.6	55
97	CO₂capture in poly(ionic liquid) membranes: atomistic insight into the role of anions. Physical Chemistry Chemical Physics, 2013, 15, 651-658.	2.8	55
98	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.	8.2	55
99	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.	8.2	55
100	Experimental and computational approach of understanding the gas adsorption in amino functionalized interpenetrated metal organic frameworks (MOFs). Journal of Materials Chemistry, 2011, 21, 17737.	6.7	54
101	Computational Design of 2D Covalent-Organic Framework Membranes for Organic Solvent Nanofiltration. ACS Sustainable Chemistry and Engineering, 2019, 7, 1734-1744.	6.7	52
102	Development of a Density Functional Theory in Three-Dimensional Nanoconfined Space: H₂ Storage in Metalâ^'Organic Frameworks. Journal of Physical Chemistry B, 2009, 113, 12326-12331.	2.6	50
103	Chiral Phosphoric Acids in Metalâ€“Organic Frameworks with Enhanced Acidity and Tunable Catalytic Selectivity. Angewandte Chemie - International Edition, 2019, 58, 14748-14757.	13.8	50
104	A molecular simulation protocol for swelling and organic solvent nanofiltration of polymer membranes. Journal of Membrane Science, 2019, 573, 639-646.	8.2	50
105	Polymers of intrinsic microporosity for gas permeation: a molecular simulation study. Molecular Simulation, 2010, 36, 992-1003.	2.0	49
106	Mechanistic insight into highly efficient gas permeation and separation in a shape-persistent ladder polymer membrane. Physical Chemistry Chemical Physics, 2014, 16, 6075.	2.8	49
107	Molecular Insight into Adsorption and Diffusion of Alkane Isomer Mixtures in Metalâ^'Organic Frameworks. Journal of Physical Chemistry B, 2009, 113, 9129-9136.	2.6	48
108	Biofuel purification by pervaporation and vapor permeation in metalâ€“organic frameworks: a computational study. Energy and Environmental Science, 2011, 4, 2107.	30.8	48

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109	Molecular insight into cellulose regeneration from a cellulose/ionic liquid mixture: effects of water concentration and temperature. RSC Advances, 2013, 3, 4425.	3.6	48
110	Confinementâ€Driven Enantioselectivity in 3D Porous Chiral Covalent Organic Frameworks. Angewandte Chemie - International Edition, 2021, 60, 6086-6093.	13.8	48
111	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.	8.0	48
112	Equation of State for the Vaporâ€'Liquid Equilibria of Binary Systems Containing Imidazolium-Based Ionic Liquids. Industrial & Engineering Chemistry Research, 2007, 46, 4323-4329.	3.7	46
113	Mechanistic understanding of interactions between cellulose and ionic liquids: A molecular simulation study. Polymer, 2011, 52, 5904-5911.	3.8	46
114	Criticality and phase behavior in the restricted-primitive model electrolyte: Description of ion association. Journal of Chemical Physics, 2002, 116, 7977-7982.	3.0	45
115	Hydrophobic Shielding of Outer Surface: Enhancing the Chemical Stability of Metalâ€“Organic Polyhedra. Angewandte Chemie - International Edition, 2019, 58, 1041-1045.	13.8	45
116	HM-IE:â€‰ Quantum Chemical Hybrid Methods for Calculating Interaction Energies. Journal of Physical Chemistry A, 2004, 108, 107-112.	2.5	44
117	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.	3.1	44
118	CO2 capture in cation-exchanged metalâ€“organic frameworks: Holistic modeling from molecular simulation to process optimization. Chemical Engineering Science, 2015, 124, 70-78.	3.8	44
119	In silico screening and design strategies of ethaneâ€selective metalâ€“organic frameworks for ethane/ethylene separation. AICHE Journal, 2021, 67, e17025.	3.6	44
120	Cation Characterization and CO2Capture in Li+-Exchanged Metalâ€'Organic Frameworks: From First-Principles Modeling to Molecular Simulationâ€. Industrial & Engineering Chemistry Research, 2011, 50, 62-68.	3.7	43
121	Porous organic cages as synthetic water channels. Nature Communications, 2020, 11, 4927.	12.8	43
122	Critical temperatures and pressures for hydrocarbon mixtures from an equation of state with renormalization-group theory corrections. Fluid Phase Equilibria, 2000, 169, 127-147.	2.5	42
123	Assessment of biomolecular force fields for molecular dynamics simulations in a protein crystal. Journal of Computational Chemistry, 2010, 31, 371-380.	3.3	42
124	Propylene/Propane Separation Using SiCHA. Industrial & Engineering Chemistry Research, 2013, 52, 3877-3892.	3.7	41
125	Nanostructural Control Enables Optimized Photoacousticâ€“Fluorescenceâ€“Magnetic Resonance Multimodal Imaging and Photothermal Therapy of Brain Tumor. Advanced Functional Materials, 2020, 30, 1907077.	14.9	41
126	Phase equilibria for chain-fluid mixtures near to and far from the critical region. AICHE Journal, 2000, 46, 2525-2536.	3.6	39

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127	Characterization of hexavalent chromium interaction with Sargassum by X-ray absorption fine structure spectroscopy, X-ray photoelectron spectroscopy, and quantum chemistry calculation. Journal of Colloid and Interface Science, 2011, 356, 741-748.	9.4	39
128	Synthesis, characterization and capacitive performance of hydrous manganese dioxide nanostructures. Nanotechnology, 2011, 22, 125703.	2.6	39
129	CO₂ Adsorption in Mono-, Di- and Trivalent Cation-Exchanged Metalâ€“Organic Frameworks: A Molecular Simulation Study. Langmuir, 2012, 28, 3903-3910.	3.5	39
130	Self-Assembly of Amphiphilic Peptide (AF)₆H₅K₁₅: Coarse-Grained Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2013, 117, 9690-9698.	2.6	39
131	High-Throughput Computational Screening of Metalâ€“Organic Frameworks for Thiol Capture. Journal of Physical Chemistry C, 2017, 121, 22208-22215.	3.1	38
132	Dendritic Ptâ€“Cu bimetallic nanocrystals with a high electrocatalytic activity toward methanol oxidation. Materials Chemistry and Physics, 2012, 132, 244-247.	4.0	37
133	Computational Characterization of Ultrathin Polymer Membranes in Liquids. Macromolecules, 2018, 51, 7169-7177.	4.8	37
134	Molecular Dynamics Simulations for Water and Ions in Protein Crystals. Langmuir, 2008, 24, 4215-4223.	3.5	36
135	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.	2.6	36
136	Molecular Design of Zirconium Tetrazolate Metalâ€“Organic Frameworks for CO₂ Capture. Crystal Growth and Design, 2017, 17, 543-549.	3.0	36
137	Polyelectrolyte solutions with stickiness between polyions and counterions. Journal of Chemical Physics, 1999, 110, 4952-4962.	3.0	35
138	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.	4.6	35
139	Highly Selective CO₂ Conversion to Methanol in a Bifunctional Zeolite Catalytic Membrane Reactor. Angewandte Chemie - International Edition, 2021, 60, 18289-18294.	13.8	35
140	Effects of Macromolecular Crowding on Biochemical Reaction Equilibria: A Molecular Thermodynamic Perspective. Biophysical Journal, 2007, 93, 1464-1473.	0.5	33
141	Efficient Removal of Pb²⁺ from Aqueous Solution by an Ionic Covalentâ€“Organic Framework: Molecular Simulation Study. Industrial & Engineering Chemistry Research, 2018, 57, 6477-6482.	3.7	33
142	Monte Carlo Simulation of O2and N2Adsorption in Nanoporous Carbon (C168Schwarzite). Langmuir, 2003, 19, 3512-3518.	3.5	32
143	Effects of Residual Solvent on Membrane Structure and Gas Permeation in a Polymer of Intrinsic Microporosity: Insight from Atomistic Simulation. Journal of Physical Chemistry C, 2011, 115, 11233-11239.	3.1	32
144	Enhancement of CO₂uptake in iso-reticular Co based zeolitic imidazolate frameworks via metal replacement. CrystEngComm, 2014, 16, 4677-4680.	2.6	32

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145	Molecular simulations in metalâ€“organic frameworks for diverse potential applications. Molecular Simulation, 2014, 40, 516-536.	2.0	31
146	Molecular Thermodynamics for Protein Precipitation with a Polyelectrolyte. Journal of Physical Chemistry B, 1999, 103, 5560-5569.	2.6	30
147	An ab Initio Study on the Effect of Carbon Surface Curvature and Ring Structure on N2(O2)â^'Carbon Intermolecular Potentials. Journal of Physical Chemistry B, 2004, 108, 9842-9851.	2.6	30
148	A generic molecular thermodynamic model for linear and branched polymer solutions in a lattice. Fluid Phase Equilibria, 2006, 244, 188-192.	2.5	29
149	Salt effect on the interactions between gemini surfactant and oppositely charged polyelectrolyte in aqueous solution. Journal of Colloid and Interface Science, 2007, 306, 405-410.	9.4	29
150	Exploration of heavy metal ions transmembrane flux enhancement across a supported liquid membrane by appropriate carrier selection. Chemical Engineering Science, 2007, 62, 6032-6039.	3.8	28
151	Atomistic Insight into Adsorption, Mobility, and Vibration of Water in Ion-Exchanged Zeolite-like Metalâ^'Organic Frameworks. ACS Nano, 2009, 3, 2563-2572.	14.6	28
152	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.	2.0	28
153	Monte Carlo Simulation of O2and N2Mixture Adsorption in Nanoporous Carbon (C168Schwarzite). Langmuir, 2003, 19, 5936-5941.	3.5	27
154	Capillary Phase Transitions of Linear and Branched Alkanes in Carbon Nanotubes from Molecular Simulation. Langmuir, 2006, 22, 7391-7399.	3.5	27
155	A new molecular thermodynamic model for multicomponent Ising lattice. Journal of Chemical Physics, 2006, 125, 164506.	3.0	27
156	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.	10.3	27
157	Zeolitic Imidazolate Framework Membranes for Organic Solvent Nanofiltration: A Molecular Simulation Exploration. ACS Applied Materials & Interfaces, 2018, 10, 33135-33143.	8.0	26
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