Jianwen Jiang

List of Publications by Year in Descending Order

270 papers	12,009 citations	61 h-index	96 g-index
285 ext. papers	13,680 ext. citations	6.9 avg, IF	7 L-index

#	Paper	IF	Citations
270	Free-standing homochiral 2D monolayers by exfoliation of molecular crystals.. *Nature*, **2022**, 602, 606-611	50.4	14
269	Growing single crystals of two-dimensional covalent organic frameworks enabled by intermediate tracing study.. *Nature Communications*, **2022**, 13, 1370	17.4	6
268	Metallated porphyrinic metal□organic frameworks for CO2 conversion to HCOOH: A computational screening and mechanistic study. *Molecular Catalysis*, **2022**, 527, 112407	3.3	1
267	Transforming CO into Methanol with N-Heterocyclic Carbene-Stabilized Coinage Metal Hydrides Immobilized in a Metal-Organic Framework UiO-68. *ACS Applied Materials & Interfaces*, **2021**,	9.5	3
266	Rapid Screening of Metal-Organic Frameworks for Propane/Propylene Separation by Synergizing Molecular Simulation and Machine Learning. *ACS Applied Materials & Interfaces*, **2021**, 13, 53454-53467	9.5	6
265	Metal□Organic Frameworks for Xylene Separation: From Computational Screening to Machine Learning. *Journal of Physical Chemistry C*, **2021**, 125, 7839-7848	3.8	6
264	Highly Selective CO2 Conversion to Methanol in a Bifunctional Zeolite Catalytic Membrane Reactor. *Angewandte Chemie*, **2021**, 133, 18437-18442	3.6	0
263	Confinement-Driven Enantioselectivity in 3D Porous Chiral Covalent Organic Frameworks. *Angewandte Chemie - International Edition*, **2021**, 60, 6086-6093	16.4	15
262	Crystalline C-C and C?C Bond-Linked Chiral Covalent Organic Frameworks. *Journal of the American Chemical Society*, **2021**, 143, 369-381	16.4	44
261	Highly Stable Zr(IV)-Based Metal-Organic Frameworks for Chiral Separation in Reversed-Phase Liquid Chromatography. *Journal of the American Chemical Society*, **2021**, 143, 390-398	16.4	42
260	Confinement-Driven Enantioselectivity in 3D Porous Chiral Covalent Organic Frameworks. *Angewandte Chemie*, **2021**, 133, 6151-6158	3.6	3
259	In silico screening and design strategies of ethane-selective metal□organic frameworks for ethane/ethylene separation. *AICHE Journal*, **2021**, 67, e17025	3.6	16
258	Concluding remarks: Cooperative phenomena in framework materials. *Faraday Discussions*, **2021**, 225, 442-454	3.6	1
257	Metal-Organic Frameworks for Liquid Phase Applications. *Advanced Science*, **2021**, 8, 2003143	13.6	8
256	Highly Selective CO Conversion to Methanol in a Bifunctional Zeolite Catalytic Membrane Reactor. *Angewandte Chemie - International Edition*, **2021**, 60, 18289-18294	16.4	8
255	Hydrogen Adsorption in Metal□Organic Framework MIL-101(Cr)□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	6.1	1
254	Highly porous nanofiber-supported monolayer graphene membranes for ultrafast organic solvent nanofiltration. *Science Advances*, **2021**, 7, eabg6263	14.3	19

253	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	9.6	44
252	Dipeptide membranes for CO2 separation: A molecular simulation study. *Fluid Phase Equilibria*, **2020**, 515, 112570	2.5	3
251	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	8.3	5
250	POC/PIM-1 mixed-matrix membranes for water desalination: A molecular simulation study. *Journal of Membrane Science*, **2020**, 608, 118173	9.6	6
249	Water Permeation through Conical Nanopores: Complex Interplay between Surface Roughness and Chemistry. *Advanced Theory and Simulations*, **2020**, 3, 2000025	3.5	4
248	Molecular simulations of liquid separations in polymer membranes. *Current Opinion in Chemical Engineering*, **2020**, 28, 66-74	5.4	10
247	Nanostructural Control Enables Optimized Photoacoustic–Fluorescence–Magnetic Resonance Multimodal Imaging and Photothermal Therapy of Brain Tumor. *Advanced Functional Materials*, **2020**, 30, 1907077	15.6	26
246	Self-Assembly of Highly Stable Zirconium(IV) Coordination Cages with Aggregation Induced Emission Molecular Rotors for Live-Cell Imaging. *Angewandte Chemie*, **2020**, 132, 10237-10245	3.6	8
245	Self-Assembly of Highly Stable Zirconium(IV) Coordination Cages with Aggregation Induced Emission Molecular Rotors for Live-Cell Imaging. *Angewandte Chemie - International Edition*, **2020**, 59, 10151-10159	16.4	55
244	Organic Small Molecule Based Photothermal Agents with Molecular Rotors for Malignant Breast Cancer Therapy. *Advanced Functional Materials*, **2020**, 30, 1907093	15.6	45
243	Porous organic cages as synthetic water channels. *Nature Communications*, **2020**, 11, 4927	17.4	17
242	Machine Learning for Polymer Swelling in Liquids. *ACS Applied Polymer Materials*, **2020**, 2, 3576-3586	4.3	5
241	Intercalation of Metal Ions into Ti3C2Tx MXene Electrodes for High-Areal-Capacitance Microsupercapacitors with Neutral Multivalent Electrolytes. *Advanced Functional Materials*, **2020**, 30, 2003721	15.6	33
240	Computational design of a metal-based frustrated Lewis pair on defective UiO-66 for CO2 hydrogenation to methanol. *Journal of Materials Chemistry A*, **2020**, 8, 22802-22815	13	7
239	Atomistic Simulation Study of Polyarylate/Zeolitic-Imidazolate Framework Mixed-Matrix Membranes for Water Desalination. *ACS Applied Nano Materials*, **2020**, 3, 10022-10031	5.6	5
238	Molecular design of chiral zirconium metal–organic frameworks for asymmetric transfer hydrogenation of imines. *Catalysis Science and Technology*, **2019**, 9, 4888-4897	5.5	2
237	A molecular simulation study for efficient separation of 2,5-furandiyldimethanamine by a microporous polyarylate membrane. *Polymer*, **2019**, 175, 8-14	3.9	4
236	Enhancing water permeation through alumina membranes by changing from cylindrical to conical nanopores. *Nanoscale*, **2019**, 11, 9869-9878	7.7	18

235	Identifying the best metal–organic frameworks and unravelling different mechanisms for the separation of pentane isomers. *Molecular Systems Design and Engineering*, **2019**, 4, 609-615	4.6	7
234	Chiral BINOL-Based Covalent Organic Frameworks for Enantioselective Sensing. *Journal of the American Chemical Society*, **2019**, 141, 7081-7089	16.4	131
233	Computational screening of metal–organic frameworks for CO2 separation. *Current Opinion in Green and Sustainable Chemistry*, **2019**, 16, 57-64	7.9	10
232	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	14.7	10
231	Effects of functionalization on the nanofiltration performance of PIM-1: Molecular simulation investigation. *Journal of Membrane Science*, **2019**, 591, 117357	9.6	11
230	Chiral Phosphoric Acids in Metal-Organic Frameworks with Enhanced Acidity and Tunable Catalytic Selectivity. *Angewandte Chemie - International Edition*, **2019**, 58, 14748-14757	16.4	24
229	Boosting Enantioselectivity of Chiral Organocatalysts with Ultrathin Two-Dimensional Metal-Organic Framework Nanosheets. *Journal of the American Chemical Society*, **2019**, 141, 17685-17695	16.4	88
228	Formation of CH Hydrate in a Mesoporous Metal-Organic Framework MIL-101: Mechanistic Insights from Microsecond Molecular Dynamics Simulations. *Journal of Physical Chemistry Letters*, **2019**, 10, 7002-7008	6.4	18
227	Microporous benzimidazole-linked polymer and its derivatives for organic solvent nanofiltration. *Polymer*, **2019**, 185, 121932	3.9	7
226	Chiral Phosphoric Acids in Metal–Organic Frameworks with Enhanced Acidity and Tunable Catalytic Selectivity. *Angewandte Chemie*, **2019**, 131, 14890-14899	3.6	10
225	Post-synthesis of a covalent organic framework nanofiltration membrane for highly efficient water treatment. *Journal of Materials Chemistry A*, **2019**, 7, 24205-24210	13	52
224	Molecular Design of Microporous Polymer Membranes for the Upgrading of Natural Gas. *Journal of Physical Chemistry C*, **2019**, 123, 6607-6615	3.8	8
223	A molecular simulation protocol for swelling and organic solvent nanofiltration of polymer membranes. *Journal of Membrane Science*, **2019**, 573, 639-646	9.6	29
222	Computational Design of 2D Covalent-Organic Framework Membranes for Organic Solvent Nanofiltration. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 1734-1744	8.3	33
221	A molecular simulation protocol for membrane pervaporation. *Journal of Membrane Science*, **2019**, 572, 676-682	9.6	8
220	Hydrophobic Shielding of Outer Surface: Enhancing the Chemical Stability of Metal–Organic Polyhedra. *Angewandte Chemie*, **2019**, 131, 1053-1057	3.6	7
219	Restriction of Molecular Rotors in Ultrathin Two-Dimensional Covalent Organic Framework Nanosheets for Sensing Signal Amplification. *Chemistry of Materials*, **2019**, 31, 146-160	9.6	75
218	Hydrophobic Shielding of Outer Surface: Enhancing the Chemical Stability of Metal-Organic Polyhedra. *Angewandte Chemie - International Edition*, **2019**, 58, 1041-1045	16.4	31

217	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	3.3	18
216	Porous organic cages embedded in a lipid membrane for water desalination: A molecular simulation study. *Journal of Membrane Science*, **2019**, 573, 177-183	9.6	11
215	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	3.6	7
214	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	16.4	88
213	Dipeptide Crystals as Reverse Osmosis Membranes for Water Desalination: Atomistic Simulation. *Journal of Physical Chemistry C*, **2018**, 122, 6026-6032	3.8	7
212	Efficient Removal of Pb2+ from Aqueous Solution by an Ionic Covalent□Organic Framework: Molecular Simulation Study. *Industrial & Engineering Chemistry Research*, **2018**, 57, 6477-6482	3.9	25
211	High-throughput computational screening of metal-organic framework membranes for upgrading of natural gas. *Journal of Membrane Science*, **2018**, 551, 47-54	9.6	53
210	Amorphous Porous Organic Cage Membranes for Water Desalination. *Journal of Physical Chemistry C*, **2018**, 122, 1732-1740	3.8	14
209	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	11.5	107
208	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	9.6	35
207	Solvent nanofiltration through polybenzimidazole membranes: Unravelling the role of pore size from molecular simulations. *Journal of Membrane Science*, **2018**, 564, 782-787	9.6	12
206	Decomposition of CH4 hydrate: effects of temperature and salt from molecular simulations. *Molecular Simulation*, **2018**, 44, 1220-1228	2	5
205	Hochfluss-Hochselektivitäts-MOF-Membran: Getränderte MIL-160-Schicht für die Trennung der Xylolisomere durch Pervaporation. *Angewandte Chemie*, **2018**, 130, 15580-15584	3.6	8
204	Molecular Simulation and Analysis of Sorption Process toward Theoretical Prediction for Liquid Permeation through Membranes. *Journal of Physical Chemistry B*, **2018**, 122, 12211-12218	3.4	5
203	High-Flux High-Selectivity Metal-Organic Framework MIL-160 Membrane for Xylene Isomer Separation by Pervaporation. *Angewandte Chemie - International Edition*, **2018**, 57, 15354-15358	16.4	52
202	Design and self-assembly of hexahedral coordination cages for cascade reactions. *Nature Communications*, **2018**, 9, 4423	17.4	49
201	Zeolitic Imidazolate Framework Membranes for Organic Solvent Nanofiltration: A Molecular Simulation Exploration. *ACS Applied Materials & Interfaces*, **2018**, 10, 33135-33143	9.5	16
200	Computational Characterization of Ultrathin Polymer Membranes in Liquids. *Macromolecules*, **2018**, 51, 7169-7177	5.5	22

199	Computational screening of hydrophobic metal–organic frameworks for the separation of H2S and CO2 from natural gas. *Journal of Materials Chemistry A*, **2018**, 6, 18898-18905	13	52
198	Chiral NH-Controlled Supramolecular Metallacycles. *Journal of the American Chemical Society*, **2017**, 139, 1554-1564	16.4	94
197	Reversed thermo-switchable molecular sieving membranes composed of two-dimensional metal-organic nanosheets for gas separation. *Nature Communications*, **2017**, 8, 14460	17.4	290
196	Water Desalination through a Zeolitic Imidazolate Framework Membrane by Electro- and Thermo-Osmosis: Which Could Be More Efficient?. *ChemistrySelect*, **2017**, 2, 3981-3986	1.8	4
195	What are the key factors governing the nucleation of CO hydrate?. *Physical Chemistry Chemical Physics*, **2017**, 19, 15657-15661	3.6	43
194	Computational design of 2D functional covalent–organic framework membranes for water desalination. *Environmental Science: Water Research and Technology*, **2017**, 3, 735-743	4.2	48
193	Porous organic cage membranes for water desalination: a simulation exploration. *Physical Chemistry Chemical Physics*, **2017**, 19, 18178-18185	3.6	18
192	Molecular Design of Zirconium Tetrazolate Metal–Organic Frameworks for CO2 Capture. *Crystal Growth and Design*, **2017**, 17, 543-549	3.5	25
191	1D-2D-3D Transformation Synthesis of Hierarchical Metal-Organic Framework Adsorbent for Multicomponent Alkane Separation. *Journal of the American Chemical Society*, **2017**, 139, 819-828	16.4	54
190	Ultrathin two-dimensional porous organic nanosheets with molecular rotors for chemical sensing. *Nature Communications*, **2017**, 8, 1142	17.4	119
189	CH Hydrate Formation between Silica and Graphite Surfaces: Insights from Microsecond Molecular Dynamics Simulations. *Langmuir*, **2017**, 33, 11956-11967	4	48
188	High-Throughput Computational Screening of Metal–Organic Frameworks for Thiol Capture. *Journal of Physical Chemistry C*, **2017**, 121, 22208-22215	3.8	25
187	Ethanolamine Purification by Nanofiltration through PIM-1 and Carbon Membranes: A Molecular Simulation Study. *Journal of Physical Chemistry C*, **2017**, 121, 20539-20545	3.8	9
186	Dipeptides Embedded in a Lipid Bilayer Membrane as Synthetic Water Channels. *Langmuir*, **2017**, 33, 11490-11495	4	3
185	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	3.8	22
184	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	3.8	51
183	A helical peptide confined in metal-organic frameworks: Microscopic insight from molecular simulation. *Microporous and Mesoporous Materials*, **2016**, 232, 138-142	5.3	6
182	Modulated Hydrothermal Synthesis of UiO-66(Hf)-Type Metal-Organic Frameworks for Optimal Carbon Dioxide Separation. *Inorganic Chemistry*, **2016**, 55, 1134-41	5.1	117

181	Synthesis and seawater desalination of molecular sieving zeolitic imidazolate framework membranes. *Desalination*, **2016**, 385, 75-82	10.3	98
180	In silico screening of 4764 computation-ready, experimental metal□organic frameworks for CO2 separation. *Journal of Materials Chemistry A*, **2016**, 4, 2105-2114	13	84
179	Design of amine-functionalized metal-organic frameworks for CO2 separation: the more amine, the better?. *Chemical Communications*, **2016**, 52, 974-7	5.8	62
178	Ibuprofen loading and release in amphiphilic peptide FA32 and its derivatives: a coarse-grained molecular dynamics simulation study. *Molecular Simulation*, **2016**, 42, 679-687	2	8
177	Seawater Pervaporation through Zeolitic Imidazolate Framework Membranes: Atomistic Simulation Study. *ACS Applied Materials & Interfaces*, **2016**, 8, 13392-9	9.5	54
176	High-throughput computational screening of 137953 metal□organic frameworks for membrane separation of a CO2/N2/CH4 mixture. *Journal of Materials Chemistry A*, **2016**, 4, 15904-15912	13	70
175	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	5.5	38
174	CO2 capture in rht metal□organic frameworks: multiscale modeling from molecular simulation to breakthrough prediction. *Journal of Materials Chemistry A*, **2015**, 3, 16327-16336	13	15
173	Water Desalination through Zeolitic Imidazolate Framework Membranes: Significant Role of Functional Groups. *Langmuir*, **2015**, 31, 13230-7	4	77
172	Cellulose dissolution and regeneration in ionic liquids: A computational perspective. *Chemical Engineering Science*, **2015**, 121, 180-189	4.4	83
171	CO 2 capture in cation-exchanged metal□organic frameworks: Holistic modeling from molecular simulation to process optimization. *Chemical Engineering Science*, **2015**, 124, 70-78	4.4	35
170	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. 4/2015). *Advanced Functional Materials*, **2015**, 25, 498-498	15.6	1
169	Computer Simulations of Ionic Metal□Organic Frameworks **2015**, 451-481		
168	Glucose recovery from aqueous solutions by adsorption in metal-organic framework MIL-101: a molecular simulation study. *Scientific Reports*, **2015**, 5, 12821	4.9	10
167	Biofuel purification in GME zeolitic□imidazolate frameworks: From ab initio calculations to molecular simulations. *AICHE Journal*, **2015**, 61, 2763-2775	3.6	16
166	Computational Amphiphilic Materials for Drug Delivery. *Frontiers in Materials*, **2015**, 2,	4	17
165	Submicrometer-Sized ZIF-71 Filled Organophilic Membranes for Improved Bioethanol Recovery: Mechanistic Insights by Monte Carlo Simulation and FTIR Spectroscopy. *Advanced Functional Materials*, **2015**, 25, 516-525	15.6	78
164	Mechanistic insight into highly efficient gas permeation and separation in a shape-persistent ladder polymer membrane. *Physical Chemistry Chemical Physics*, **2014**, 16, 6075-83	3.6	38

163	Synthesis of highly hydrophobic and permselective metal–organic framework Zn(BDC)(TED)0.5 membranes for H2/CO2 separation. *Journal of Membrane Science*, **2014**, 454, 126-132	9.6	47
162	Enhancement of CO2 uptake in iso-reticular Co based zeolitic imidazolate frameworks via metal replacement. *CrystEngComm*, **2014**, 16, 4677-4680	3.3	28
161	Covalent-organic framework as a template to assemble carbon nanotubes into a high-density membrane: computational demonstration. *Nanoscale*, **2014**, 6, 772-7	7.7	4
160	Molecular simulations in metal–organic frameworks for diverse potential applications. *Molecular Simulation*, **2014**, 40, 516-536	2	29
159	Self-assembly of amphiphilic peptide (AF)6H5K15 derivatives: roles of hydrophilic and hydrophobic residues. *Journal of Physical Chemistry B*, **2014**, 118, 2683-92	3.4	18
158	A combinatorial approach towards water-stable metal-organic frameworks for highly efficient carbon dioxide separation. *ChemSusChem*, **2014**, 7, 2791-5	8.3	68
157	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	3.8	112
156	"Click"-extended nitrogen-rich metal-organic frameworks and their high performance in CO2-selective capture. *Chemical Communications*, **2014**, 50, 4683-5	5.8	55
155	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	3.8	37
154	Engineering chiral porous metal-organic frameworks for enantioselective adsorption and separation. *Nature Communications*, **2014**, 5, 4406	17.4	183
153	Biofuel purification in zeolitic imidazolate frameworks: the significant role of functional groups. *Physical Chemistry Chemical Physics*, **2014**, 16, 9643-55	3.6	48
152	Molecular insights into the self-assembly of short amphiphilic peptides FmDn and FmKn. *RSC Advances*, **2014**, 4, 60741-60748	3.7	7
151	Crucial role of blocking inaccessible cages in the simulation of gas adsorption in a paddle-wheel metal–organic framework. *RSC Advances*, **2013**, 3, 16152	3.7	12
150	Self-assembly of amphiphilic peptide (AF)6H5K15: coarse-grained molecular dynamics simulation. *Journal of Physical Chemistry B*, **2013**, 117, 9690-8	3.4	31
149	Adsorption of C1–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	3.8	60
148	Ag nanoprisms with Ag2S attachment. *Scientific Reports*, **2013**, 3, 2177	4.9	52
147	Engineering nanostructured materials for sustainable future. *Asia-Pacific Journal of Chemical Engineering*, **2013**, 8, 203-204	1.3	
146	Thermal Conductivity of Zeolitic Imidazolate Framework-8: A Molecular Simulation Study. *Journal of Physical Chemistry C*, **2013**, 117, 18441-18447	3.8	81

145	Ionic Liquid Membranes Supported by Hydrophobic and Hydrophilic Metal–Organic Frameworks for CO2 Capture. *Journal of Physical Chemistry C*, **2013**, 117, 5792-5799	3.8	68
144	Functionalized metal–organic framework MIL-101 for CO2 capture: multi-scale modeling from ab initio calculation and molecular simulation to breakthrough prediction. *CrystEngComm*, **2013**, 15, 10358	3.3	25
143	Cellulose regeneration from a cellulose/ionic liquid mixture: the role of anti-solvents. *RSC Advances*, **2013**, 3, 12794	3.7	52
142	CO2 capture in poly(ionic liquid) membranes: atomistic insight into the role of anions. *Physical Chemistry Chemical Physics*, **2013**, 15, 651-8	3.6	47
141	Liquid chromatographic separation in metal-organic framework MIL-101: a molecular simulation study. *Langmuir*, **2013**, 29, 1650-6	4	16
140	Sorption-induced structural transition of zeolitic imidazolate framework-8: a hybrid molecular simulation study. *Journal of the American Chemical Society*, **2013**, 135, 3722-8	16.4	120
139	A rationally designed nitrogen-rich metal-organic framework and its exceptionally high CO(2) and H(2) uptake capability. *Scientific Reports*, **2013**, 3, 1149	4.9	117
138	Propylene/Propane Separation Using SiCHA. *Industrial & Engineering Chemistry Research*, **2013**, 52, 3877-3892	3.9	30
137	Atomistic insight into micro-phase separation and gas diffusion in PEO–PBT multiblock copolymers. *Molecular Simulation*, **2013**, 39, 902-907	2	2
136	Molecular insight into cellulose regeneration from a cellulose/ionic liquid mixture: effects of water concentration and temperature. *RSC Advances*, **2013**, 3, 4425	3.7	34
135	Self-templated free-radical polymerization to form tactic chains in confined environment. *Journal of Physical Chemistry B*, **2013**, 117, 7826-32	3.4	1
134	Dendritic Pt–Cu bimetallic nanocrystals with a high electrocatalytic activity toward methanol oxidation. *Materials Chemistry and Physics*, **2012**, 132, 244-247	4.4	36
133	pH-sensitive drug loading/releasing in amphiphilic copolymer PAE-PEG: integrating molecular dynamics and dissipative particle dynamics simulations. *Journal of Controlled Release*, **2012**, 162, 185-93	11.7	129
132	Fluorinated metal-organic frameworks: advantageous for higher H2 and CO2 adsorption or not?. *Chemistry - A European Journal*, **2012**, 18, 688-94	4.8	86
131	CO2 adsorption in mono-, di- and trivalent cation-exchanged metal-organic frameworks: a molecular simulation study. *Langmuir*, **2012**, 28, 3903-10	4	36
130	Development of a force field for zeolitic imidazolate framework-8 with structural flexibility. *Journal of Chemical Physics*, **2012**, 136, 244703	3.9	55
129	A homochiral metal-organic framework membrane for enantioselective separation. *Chemical Communications*, **2012**, 48, 7022-4	5.8	116
128	Ion Exchange in Metal–Organic Framework for Water Purification: Insight from Molecular Simulation. *Journal of Physical Chemistry C*, **2012**, 116, 6925-6931	3.8	61

127	Metal–Organic Framework/Polymer Mixed-Matrix Membranes for H2/CO2 Separation: A Fully Atomistic Simulation Study. *Journal of Physical Chemistry C*, **2012**, 116, 19268-19277	3.8	63
126	Crowding effect on DNA melting: a molecular thermodynamic model with explicit solvent. *Physical Chemistry Chemical Physics*, **2012**, 14, 15400-5	3.6	8
125	Recent development of in silico molecular modeling for gas and liquid separations in metal–organic frameworks. *Current Opinion in Chemical Engineering*, **2012**, 1, 138-144	5.4	17
124	Recovery of dimethyl sulfoxide from aqueous solutions by highly selective adsorption in hydrophobic metal-organic frameworks. *Langmuir*, **2012**, 28, 15305-12	4	22
123	A highly permeable and selective zeolitic imidazolate framework ZIF-95 membrane for H2/CO2 separation. *Chemical Communications*, **2012**, 48, 10981-3	5.8	174
122	Metal-organic framework supported ionic liquid membranes for CO2 capture: anion effects. *Physical Chemistry Chemical Physics*, **2012**, 14, 5785-94	3.6	98
121	Bovine pancreatic trypsin inhibitor crystals with different morphologies: a molecular dynamics simulation study. *Molecular Simulation*, **2012**, 38, 112-118	2	0
120	Amino functionalized zeolitic tetrazolate framework (ZTF) with high capacity for storage of carbon dioxide. *Chemical Communications*, **2011**, 47, 2011-3	5.8	204
119	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	3.8	51
118	Molecular simulations for energy, environmental and pharmaceutical applications of nanoporous materials: from zeolites, metal-organic frameworks to protein crystals. *Chemical Society Reviews*, **2011**, 40, 3599-612	58.5	113
117	Zeolitic imidazolate framework-8 as a reverse osmosis membrane for water desalination: insight from molecular simulation. *Journal of Chemical Physics*, **2011**, 134, 134705	3.9	153
116	Effects of polydisperse crowders on aggregation reactions: a molecular thermodynamic analysis. *Journal of Chemical Physics*, **2011**, 134, 064704	3.9	8
115	Ionic Liquid/Metal–Organic Framework Composite for CO2 Capture: A Computational Investigation. *Journal of Physical Chemistry C*, **2011**, 115, 21736-21742	3.8	99
114	Structural Isomerism and Effect of Fluorination on Gas Adsorption in Copper-Tetrazolate Based Metal Organic Frameworks. *Chemistry of Materials*, **2011**, 23, 2908-2916	9.6	73
113	Synthesis and Capacitive Properties of Manganese Oxide Nanosheets Dispersed on Functionalized Graphene Sheets. *Journal of Physical Chemistry C*, **2011**, 115, 6448-6454	3.8	332
112	A high-performance asymmetric supercapacitor fabricated with graphene-based electrodes. *Energy and Environmental Science*, **2011**, 4, 4009	35.4	666
111	Mechanistic understanding of interactions between cellulose and ionic liquids: A molecular simulation study. *Polymer*, **2011**, 52, 5904-5911	3.9	43
110	Experimental and computational approach of understanding the gas adsorption in amino functionalized interpenetrated metal organic frameworks (MOFs). *Journal of Materials Chemistry*, **2011**, 21, 17737		48

109	DNA melting in slit pores: a reaction density functional theory. *Journal of Physical Chemistry B*, **2011**, 115, 1848-55	3.4	4
108	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	3.8	28
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