Jianwen Jiang

List of Publications by Citations

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	A high-performance asymmetric supercapacitor fabricated with graphene-based electrodes. *Energy and Environmental Science*, **2011**, 4, 4009	35.4	666
269	Storage and separation of CO2 and CH4 in silicalite, C168 schwarzite, and IRMOF-1: a comparative study from Monte Carlo simulation. *Langmuir*, **2007**, 23, 659-66	4	358
268	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
267	Reversed thermo-switchable molecular sieving membranes composed of two-dimensional metal-organic nanosheets for gas separation. *Nature Communications*, **2017**, 8, 14460	17.4	290
266	Molecular screening of metal-organic frameworks for CO2 storage. *Langmuir*, **2008**, 24, 6270-8	4	221
265	Amino functionalized zeolitic tetrazolate framework (ZTF) with high capacity for storage of carbon dioxide. *Chemical Communications*, **2011**, 47, 2011-3	5.8	204
264	Unprecedentedly high selective adsorption of gas mixtures in rho zeolite-like metal-organic framework: a molecular simulation study. *Journal of the American Chemical Society*, **2009**, 131, 11417-25	16.4	196
263	Engineering chiral porous metal-organic frameworks for enantioselective adsorption and separation. *Nature Communications*, **2014**, 5, 4406	17.4	183
262	A highly permeable and selective zeolitic imidazolate framework ZIF-95 membrane for H2/CO2 separation. *Chemical Communications*, **2012**, 48, 10981-3	5.8	174
261	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
260	Molecular dynamics and dissipative particle dynamics simulations for the miscibility of poly(ethylene oxide)/poly(vinyl chloride) blends. *Polymer*, **2010**, 51, 291-299	3.9	138
259	Chiral BINOL-Based Covalent Organic Frameworks for Enantioselective Sensing. *Journal of the American Chemical Society*, **2019**, 141, 7081-7089	16.4	131
258	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
257	Molecular simulations for adsorptive separation of CO2/CH4 mixture in metal-exposed, catenated, and charged metal-organic frameworks. *Langmuir*, **2009**, 25, 5239-47	4	126
256	Diffusion and separation of CO2 and CH4 in silicalite, C168 schwarzite, and IRMOF-1: a comparative study from molecular dynamics simulation. *Langmuir*, **2008**, 24, 5474-84	4	125
255	Template Synthesis of Tubular Ruthenium Oxides for Supercapacitor Applications. *Journal of Physical Chemistry C*, **2010**, 114, 13608-13613	3.8	121
254	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

253	Ultrathin two-dimensional porous organic nanosheets with molecular rotors for chemical sensing. *Nature Communications*, **2017**, 8, 1142	17.4	119
252	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
251	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
250	A homochiral metal-organic framework membrane for enantioselective separation. *Chemical Communications*, **2012**, 48, 7022-4	5.8	116
249	Monte Carlo simulation for the adsorption and separation of linear and branched alkanes in IRMOF-1. *Langmuir*, **2006**, 22, 5702-7	4	116
248	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
247	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
246	Exceptionally high CO2storage in covalent-organic frameworks: Atomistic simulation study. *Energy and Environmental Science*, **2008**, 1, 139	35.4	111
245	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
244	Metal-organic framework MIL-101 for adsorption and effect of terminal water molecules: from quantum mechanics to molecular simulation. *Langmuir*, **2010**, 26, 8743-50	4	102
243	Ionic Liquid/Metal□Organic Framework Composite for CO2 Capture: A Computational Investigation. *Journal of Physical Chemistry C*, **2011**, 115, 21736-21742	3.8	99
242	Molecular Understanding for the Adsorption of Water and Alcohols in Hydrophilic and Hydrophobic Zeolitic Metal□Organic Frameworks. *Journal of Physical Chemistry C*, **2010**, 114, 11542-11550	3.8	99
241	Synthesis and seawater desalination of molecular sieving zeolitic imidazolate framework membranes. *Desalination*, **2016**, 385, 75-82	10.3	98
240	Metal-organic framework supported ionic liquid membranes for CO2 capture: anion effects. *Physical Chemistry Chemical Physics*, **2012**, 14, 5785-94	3.6	98
239	Chiral NH-Controlled Supramolecular Metallacycles. *Journal of the American Chemical Society*, **2017**, 139, 1554-1564	16.4	94
238	A Highly Hydrophobic Metal□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	3.8	90
237	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
236	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

235	A bio-metal-organic framework for highly selective CO(2) capture: A molecular simulation study. *ChemSusChem*, **2010**, 3, 982-8	8.3	88
234	Equation of state for thermodynamic properties of chain fluids near-to and far-from the vapor□quid critical region. *Journal of Chemical Physics*, **1999**, 111, 5964-5974	3.9	87
233	Fluorinated metal-organic frameworks: advantageous for higher H2 and CO2 adsorption or not?. *Chemistry - A European Journal*, **2012**, 18, 688-94	4.8	86
232	In silico screening of 4764 computation-ready, experimental metal□rganic frameworks for CO2 separation. *Journal of Materials Chemistry A*, **2016**, 4, 2105-2114	13	84
231	Cellulose dissolution and regeneration in ionic liquids: A computational perspective. *Chemical Engineering Science*, **2015**, 121, 180-189	4.4	83
230	Adsorption and separation of linear and branched alkanes on carbon nanotube bundles from configurational-bias Monte Carlo simulation. *Physical Review B*, **2005**, 72,	3.3	82
229	Thermal Conductivity of Zeolitic Imidazolate Framework-8: A Molecular Simulation Study. *Journal of Physical Chemistry C*, **2013**, 117, 18441-18447	3.8	81
228	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
227	Water Desalination through Zeolitic Imidazolate Framework Membranes: Significant Role of Functional Groups. *Langmuir*, **2015**, 31, 13230-7	4	77
226	Unraveling the Energetics and Dynamics of Ibuprofen in Mesoporous Metal□rganic Frameworks. *Journal of Physical Chemistry C*, **2009**, 113, 18287-18291	3.8	77
225	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
224	Effects of Solvent Viscosity on Protein Dynamics: Infrared Vibrational Echo Experiments and Theory. *Journal of Physical Chemistry B*, **2001**, 105, 1081-1092	3.4	74
223	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
222	Separation of CO2 and N2 by adsorption in C168 schwarzite: a combination of quantum mechanics and molecular simulation study. *Journal of the American Chemical Society*, **2005**, 127, 11989-97	16.4	73
221	Highly porous ionic rht metal-organic framework for H2 and CO2 storage and separation: a molecular simulation study. *Langmuir*, **2010**, 26, 11196-203	4	71
220	High-throughput computational screening of 137953 metal□rganic frameworks for membrane separation of a CO2/N2/CH4 mixture. *Journal of Materials Chemistry A*, **2016**, 4, 15904-15912	13	70
219	A combinatorial approach towards water-stable metal-organic frameworks for highly efficient carbon dioxide separation. *ChemSusChem*, **2014**, 7, 2791-5	8.3	68
218	Ionic Liquid Membranes Supported by Hydrophobic and Hydrophilic Metal□rganic Frameworks for CO2 Capture. *Journal of Physical Chemistry C*, **2013**, 117, 5792-5799	3.8	68

217	Capillary Phase Transitions of n-Alkanes in a Carbon Nanotube. *Nano Letters*, **2004**, 4, 241-244	11.5	65
216	Upgrade of natural gas in rhozeolite-like metal□organic framework and effect of water: a computational study. *Energy and Environmental Science*, **2009**, 2, 1088	35.4	64
215	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
214	A molecular-thermodynamic model for polyelectrolyte solutions. *Journal of Chemical Physics*, **1998**, 108, 780-784	3.9	63
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212	Interactions between bovine serum albumin and gemini surfactant alkanediyl-alpha, omega-bis(dimethyldodecyl-ammonium bromide). *Biopolymers*, **2006**, 83, 243-9	2.2	62
211	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
210	Nitrogen and oxygen mixture adsorption on carbon nanotube bundles from molecular simulation. *Langmuir*, **2004**, 20, 10910-8	4	61
209	Adsorption of C1□4 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
208	Nitrogen adsorption on carbon nanotube bundles: Role of the external surface. *Physical Review B*, **2003**, 68,	3.3	59
207	Thermodynamic properties and phase equilibria of charged hard sphere chain model for polyelectrolyte solutions. *Molecular Physics*, **2001**, 99, 1121-1128	1.7	59
206	Density functional theory for adsorption of gas mixtures in metal-organic frameworks. *Journal of Physical Chemistry B*, **2010**, 114, 2820-7	3.4	56
205	"Click"-extended nitrogen-rich metal-organic frameworks and their high performance in CO2-selective capture. *Chemical Communications*, **2014**, 50, 4683-5	5.8	55
204	Development of a force field for zeolitic imidazolate framework-8 with structural flexibility. *Journal of Chemical Physics*, **2012**, 136, 244703	3.9	55
203	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
202	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
201	Mechanistic understanding of CO2-induced plasticization of a polyimide membrane: A combination of experiment and simulation study. *Polymer*, **2010**, 51, 4439-4447	3.9	54
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198	A New Model for the Viscosity of Electrolyte Solutions. *Industrial & Engineering Chemistry Research*, **2003**, 42, 6267-6272	3.9	53
197	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
196	Ag nanoprisms with Ag attachment. *Scientific Reports*, **2013**, 3, 2177	4.9	52
195	Cellulose regeneration from a cellulose/ionic liquid mixture: the role of anti-solvents. *RSC Advances*, **2013**, 3, 12794	3.7	52
194	Charged soc metal-organic framework for high-efficacy H2 adsorption and syngas purification: Atomistic simulation study. *AICHE Journal*, **2009**, 55, 2422-2432	3.6	52
193	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
192	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
191	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
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188	Design and self-assembly of hexahedral coordination cages for cascade reactions. *Nature Communications*, **2018**, 9, 4423	17.4	49
187	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
186	CH Hydrate Formation between Silica and Graphite Surfaces: Insights from Microsecond Molecular Dynamics Simulations. *Langmuir*, **2017**, 33, 11956-11967	4	48
185	Biofuel purification in zeolitic imidazolate frameworks: the significant role of functional groups. *Physical Chemistry Chemical Physics*, **2014**, 16, 9643-55	3.6	48
184	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
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182	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

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180	Development of a density functional theory in three-dimensional nanoconfined space: H2 storage in metal-organic frameworks. *Journal of Physical Chemistry B*, **2009**, 113, 12326-31	3.4	46
179	Organic Small Molecule Based Photothermal Agents with Molecular Rotors for Malignant Breast Cancer Therapy. *Advanced Functional Materials*, **2020**, 30, 1907093	15.6	45
178	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
177	Equation of State for the Vapor□liquid Equilibria of Binary Systems Containing Imidazolium-Based Ionic Liquids. *Industrial & Engineering Chemistry Research*, **2007**, 46, 4323-4329	3.9	44
176	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
175	What are the key factors governing the nucleation of CO hydrate?. *Physical Chemistry Chemical Physics*, **2017**, 19, 15657-15661	3.6	43
174	Mechanistic understanding of interactions between cellulose and ionic liquids: A molecular simulation study. *Polymer*, **2011**, 52, 5904-5911	3.9	43
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172	HM-IE: Quantum Chemical Hybrid Methods for Calculating Interaction Energies. *Journal of Physical Chemistry A*, **2004**, 108, 107-112	2.8	43
171	Criticality and phase behavior in the restricted-primitive model electrolyte: Description of ion association. *Journal of Chemical Physics*, **2002**, 116, 7977-7982	3.9	42
170	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
169	Cation Characterization and CO2Capture in Li+-Exchanged Metal□Organic Frameworks: From First-Principles Modeling to Molecular Simulation□ *Industrial & Engineering Chemistry Research*, **2011**, 50, 62-68	3.9	41
168	Polymers of intrinsic microporosity for gas permeation: a molecular simulation study. *Molecular Simulation*, **2010**, 36, 992-1003	2	40
167	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	39
166	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
165	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
164	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

163	Dendritic PtCu bimetallic nanocrystals with a high electrocatalytic activity toward methanol oxidation. *Materials Chemistry and Physics*, **2012**, 132, 244-247	4.4	36
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161	Synthesis, characterization and capacitive performance of hydrous manganese dioxide nanostructures. *Nanotechnology*, **2011**, 22, 125703	3.4	36
160	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
159	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
158	Phase equilibria for chain-fluid mixtures near to and far from the critical region. *AICHE Journal*, **2000**, 46, 2525-2536	3.6	35
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154	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
153	Computational Design of 2D Covalent-Organic Framework Membranes for Organic Solvent Nanofiltration. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 1734-1744	8.3	33
152	Self-assembly of amphiphilic peptide (AF)6H5K15: coarse-grained molecular dynamics simulation. *Journal of Physical Chemistry B*, **2013**, 117, 9690-8	3.4	31
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150	Hydrophobic Shielding of Outer Surface: Enhancing the Chemical Stability of Metal-Organic Polyhedra. *Angewandte Chemie - International Edition*, **2019**, 58, 1041-1045	16.4	31
149	Propylene/Propane Separation Using SiCHA. *Industrial & Engineering Chemistry Research*, **2013**, 52, 3877-3892	3.9	30
148	Assessment of biomolecular force fields for molecular dynamics simulations in a protein crystal. *Journal of Computational Chemistry*, **2010**, 31, 371-80	3.5	30
147	Monte Carlo Simulation of O2 and N2 Adsorption in Nanoporous Carbon (C168 Schwarzite). *Langmuir*, **2003**, 19, 3512-3518	4	30
146	Molecular simulations in metal-organic frameworks for diverse potential applications. *Molecular Simulation*, **2014**, 40, 516-536	2	29

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144	Molecular Thermodynamics for Protein Precipitation with a Polyelectrolyte. *Journal of Physical Chemistry B*, **1999**, 103, 5560-5569	3.4	29
143	A molecular simulation protocol for swelling and organic solvent nanofiltration of polymer membranes. *Journal of Membrane Science*, **2019**, 573, 639-646	9.6	29
142	Enhancement of CO2 uptake in iso-reticular Co based zeolitic imidazolate frameworks via metal replacement. *CrystEngComm*, **2014**, 16, 4677-4680	3.3	28
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136	Exploration of heavy metal ions transmembrane flux enhancement across a supported liquid membrane by appropriate carrier selection. *Chemical Engineering Science*, **2007**, 62, 6032-6039	4.4	26
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125	Recovery of dimethyl sulfoxide from aqueous solutions by highly selective adsorption in hydrophobic metal-organic frameworks. *Langmuir*, **2012**, 28, 15305-12	4	22
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123	Computational Characterization of Ultrathin Polymer Membranes in Liquids. *Macromolecules*, **2018**, 51, 7169-7177	5.5	22
122	An experimental evaluation and molecular simulation of high temperature gas adsorption on nanoporous carbon. *Carbon*, **2011**, 49, 117-125	10.4	21
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120	Recognition of multiblock copolymers on nanopatterned surfaces: insight from molecular simulations. *Langmuir*, **2007**, 23, 2430-6	4	21
119	Experimental and computational studies of membrane extraction of Cu(II). *AICHE Journal*, **2006**, 52, 3266-3277	3.6	21
118	Phase behavior of polyampholytes from charged hard-sphere chain model. *Journal of Chemical Physics*, **2006**, 124, 144908	3.9	19
117	Highly porous nanofiber-supported monolayer graphene membranes for ultrafast organic solvent nanofiltration. *Science Advances*, **2021**, 7, eabg6263	14.3	19
116	Porous organic cage membranes for water desalination: a simulation exploration. *Physical Chemistry Chemical Physics*, **2017**, 19, 18178-18185	3.6	18
115	Enhancing water permeation through alumina membranes by changing from cylindrical to conical nanopores. *Nanoscale*, **2019**, 11, 9869-9878	7.7	18
114	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
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