

Kang Zhang

List of Publications by Year in descending order

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31
papers

2,167
citations

304602

22
h-index

434063

31
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32
all docs

32
docs citations

32
times ranked

3397
citing authors

#	ARTICLE	IF	CITATIONS
1	Reversed thermo-switchable molecular sieving membranes composed of two-dimensional metal-organic nanosheets for gas separation. <i>Nature Communications</i> , 2017, 8, 14460.	5.8	382
2	Engineering chiral porous metal-organic frameworks for enantioselective adsorption and separation. <i>Nature Communications</i> , 2014, 5, 4406.	5.8	221
3	Ultrathin two-dimensional porous organic nanosheets with molecular rotors for chemical sensing. <i>Nature Communications</i> , 2017, 8, 1142.	5.8	152
4	Chiral NH-Controlled Supramolecular Metallacycles. <i>Journal of the American Chemical Society</i> , 2017, 139, 1554-1564.	6.6	122
5	Confinement of Aggregation-Induced Emission Molecular Rotors in Ultrathin Two-Dimensional Porous Organic Nanosheets for Enhanced Molecular Recognition. <i>Journal of the American Chemical Society</i> , 2018, 140, 4035-4046.	6.6	119
6	In silico screening of 4764 computation-ready, experimental metal-organic frameworks for CO ₂ separation. <i>Journal of Materials Chemistry A</i> , 2016, 4, 2105-2114.	5.2	109
7	Water Desalination through Zeolitic Imidazolate Framework Membranes: Significant Role of Functional Groups. <i>Langmuir</i> , 2015, 31, 13230-13237.	1.6	108
8	Submicrometer-Sized ZIF-71 Filled Organophilic Membranes for Improved Bioethanol Recovery: Mechanistic Insights by Monte Carlo Simulation and FTIR Spectroscopy. <i>Advanced Functional Materials</i> , 2015, 25, 516-525.	7.8	94
9	A Combinatorial Approach towards Water-Stable Metal-Organic Frameworks for Highly Efficient Carbon Dioxide Separation. <i>ChemSusChem</i> , 2014, 7, 2791-2795.	3.6	82
10	Seawater Pervaporation through Zeolitic Imidazolate Framework Membranes: Atomistic Simulation Study. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 13392-13399.	4.0	72
11	Adsorption of C ₁ -C ₄ Alcohols in Zeolitic Imidazolate Framework-8: Effects of Force Fields, Atomic Charges, and Framework Flexibility. <i>Journal of Physical Chemistry C</i> , 2013, 117, 25628-25635.	1.5	70
12	Computational design of 2D functional covalent-organic framework membranes for water desalination. <i>Environmental Science: Water Research and Technology</i> , 2017, 3, 735-743.	1.2	69
13	1D-2D-3D Transformation Synthesis of Hierarchical Metal-Organic Framework Adsorbent for Multicomponent Alkane Separation. <i>Journal of the American Chemical Society</i> , 2017, 139, 819-828.	6.6	62
14	Ag nanoprisms with Ag ₂ S attachment. <i>Scientific Reports</i> , 2013, 3, 2177.	1.6	61
15	Click-extended nitrogen-rich metal-organic frameworks and their high performance in CO ₂ -selective capture. <i>Chemical Communications</i> , 2014, 50, 4683.	2.2	61
16	Biofuel purification in zeolitic imidazolate frameworks: the significant role of functional groups. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 9643-9655.	1.3	57
17	Water desalination and biofuel dehydration through a thin membrane of polymer of intrinsic microporosity: Atomistic simulation study. <i>Journal of Membrane Science</i> , 2018, 545, 49-56.	4.1	55
18	Functionalized metal-organic framework MIL-101 for CO ₂ capture: multi-scale modeling from ab initio calculation and molecular simulation to breakthrough prediction. <i>CrystEngComm</i> , 2013, 15, 10358.	1.3	36

#	ARTICLE	IF	CITATIONS
19	Molecular Design of Zirconium Tetrazolate Metal-Organic Frameworks for CO ₂ Capture. <i>Crystal Growth and Design</i> , 2017, 17, 543-549.	1.4	36
20	Formation of CH ₄ Hydrate in a Mesoporous Metal-Organic Framework MIL-101: Mechanistic Insights from Microsecond Molecular Dynamics Simulations. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7002-7008.	2.1	35
21	Efficient Removal of Pb ²⁺ from Aqueous Solution by an Ionic Covalent-Organic Framework: Molecular Simulation Study. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 6477-6482.	1.8	33
22	Molecular Dynamics Phenomena of Water in the Metalorganic Framework MIL-100(Al), as Revealed by Pulsed Field Gradient NMR and Atomistic Simulation. <i>Journal of Physical Chemistry C</i> , 2017, 121, 18065-18074.	1.5	25
23	Biofuel purification in GME zeolitic-imidazolate frameworks: From <i>ab initio</i> calculations to molecular simulations. <i>AIChE Journal</i> , 2015, 61, 2763-2775.	1.8	22
24	CO ₂ capture in metal-organic frameworks: multiscale modeling from molecular simulation to breakthrough prediction. <i>Journal of Materials Chemistry A</i> , 2015, 3, 16327-16336.	5.2	20
25	Crucial role of blocking inaccessible cages in the simulation of gas adsorption in a paddle-wheel metal-organic framework. <i>RSC Advances</i> , 2013, 3, 16152.	1.7	15
26	Functional UiO-66 for the removal of sulfur-containing compounds in gas and liquid mixtures: A molecular simulation study. <i>Chemical Engineering Journal</i> , 2019, 356, 737-745.	6.6	15
27	Diameter Effect on the Sidewall Functionalization of Single-Walled Carbon Nanotubes by Addition of Dichlorocarbene. <i>Advanced Functional Materials</i> , 2012, 22, 5216-5223.	7.8	13
28	Glucose recovery from aqueous solutions by adsorption in metal-organic framework MIL-101: a molecular simulation study. <i>Scientific Reports</i> , 2015, 5, 12821.	1.6	11
29	Molecular Simulation and Analysis of Sorption Process toward Theoretical Prediction for Liquid Permeation through Membranes. <i>Journal of Physical Chemistry B</i> , 2018, 122, 12211-12218.	1.2	7
30	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. <i>ACS Applied Energy Materials</i> , 2021, 4, 7839-7847.	2.5	2
31	Porous Materials: Submicrometer-Sized ZIF-71 Filled Organophilic Membranes for Improved Bioethanol Recovery: Mechanistic Insights by Monte Carlo Simulation and FTIR Spectroscopy (<i>Adv. Funct. Mater.</i>) Tj ETQq1 1 0.784314 ngBT /Ov	7.8	13