

Ravichandar Babarao

List of Publications by Year in descending order

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85
papers

6,829
citations

61945

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58549

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88
docs citations

88
times ranked

7705
citing authors

#	ARTICLE	IF	CITATIONS
1	Chemically Stable Multilayered Covalent Organic Nanosheets from Covalent Organic Frameworks via Mechanical Delamination. <i>Journal of the American Chemical Society</i> , 2013, 135, 17853-17861.	6.6	717
2	Phosphoric Acid Loaded Azo (âˆ•Nâ••Nâˆ•) Based Covalent Organic Framework for Proton Conduction. <i>Journal of the American Chemical Society</i> , 2014, 136, 6570-6573.	6.6	562
3	Storage and Separation of CO ₂ and CH ₄ in Silicalite, C ₁₆₈ Schwarzite, and IRMOF-1: A Comparative Study from Monte Carlo Simulation. <i>Langmuir</i> , 2007, 23, 659-666.	1.6	388
4	A Robust Ethane-Trapping Metalâ€“Organic Framework with a High Capacity for Ethylene Purification. <i>Journal of the American Chemical Society</i> , 2019, 141, 5014-5020.	6.6	272
5	Molecular Screening of Metalâˆ“Organic Frameworks for CO ₂ Storage. <i>Langmuir</i> , 2008, 24, 6270-6278.	1.6	227
6	Unprecedentedly High Selective Adsorption of Gas Mixtures in ρ Zeolite-like Metalâˆ“Organic Framework: A Molecular Simulation Study. <i>Journal of the American Chemical Society</i> , 2009, 131, 11417-11425.	6.6	202
7	A route to drastic increase of CO ₂ uptake in Zr metal organic framework UiO-66. <i>Chemical Communications</i> , 2013, 49, 3634.	2.2	201
8	Post-synthetic Structural Processing in a Metalâ€“Organic Framework Material as a Mechanism for Exceptional CO ₂ /N ₂ Selectivity. <i>Journal of the American Chemical Society</i> , 2013, 135, 10441-10448.	6.6	190
9	Selective capture of carbon dioxide from hydrocarbons using a metal-organic framework. <i>Nature Communications</i> , 2021, 12, 197.	5.8	177
10	Defect engineering of UiO-66 for CO ₂ and H ₂ O uptake â€“ a combined experimental and simulation study. <i>Dalton Transactions</i> , 2016, 45, 4496-4500.	1.6	171
11	Direct Synthesis of Hierarchically Porous Metalâ€“Organic Frameworks with High Stability and Strong Brønsted Acidity: The Decisive Role of Hafnium in Efficient and Selective Fructose Dehydration. <i>Chemistry of Materials</i> , 2016, 28, 2659-2667.	3.2	160
12	Lead(II) uptake by aluminium based magnetic framework composites (MFCs) in water. <i>Journal of Materials Chemistry A</i> , 2015, 3, 19822-19831.	5.2	141
13	Diffusion and Separation of CO ₂ and CH ₄ in Silicalite, C ₁₆₈ Schwarzite, and IRMOF-1: A Comparative Study from Molecular Dynamics Simulation. <i>Langmuir</i> , 2008, 24, 5474-5484.	1.6	140
14	Defects in metalâ€“organic frameworks: a compromise between adsorption and stability?. <i>Dalton Transactions</i> , 2016, 45, 4352-4359.	1.6	140
15	Molecular Simulations for Adsorptive Separation of CO ₂ /CH ₄ Mixture in Metal-Exposed, Catenated, and Charged Metalâˆ“Organic Frameworks. <i>Langmuir</i> , 2009, 25, 5239-5247.	1.6	134
16	Understanding the High Solubility of CO ₂ in an Ionic Liquid with the Tetracyanoborate Anion. <i>Journal of Physical Chemistry B</i> , 2011, 115, 9789-9794.	1.2	132
17	Molecular simulations for energy, environmental and pharmaceutical applications of nanoporous materials: from zeolites, metalâ€“organic frameworks to protein crystals. <i>Chemical Society Reviews</i> , 2011, 40, 3599.	18.7	130
18	Exceptionally high CO ₂ storage in covalent-organic frameworks: Atomistic simulation study. <i>Energy and Environmental Science</i> , 2008, 1, 139.	15.6	126

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19	Functionalizing Porous Aromatic Frameworks with Polar Organic Groups for High-Capacity and Selective CO ₂ Separation: A Molecular Simulation Study. <i>Langmuir</i> , 2011, 27, 3451-3460.	1.6	124
20	Multipurpose Metal-Organic Framework for the Adsorption of Acetylene: Ethylene Purification and Carbon Dioxide Removal. <i>Chemistry of Materials</i> , 2019, 31, 4919-4926.	3.2	120
21	Metal-Organic Framework MIL-101 for Adsorption and Effect of Terminal Water Molecules: From Quantum Mechanics to Molecular Simulation. <i>Langmuir</i> , 2010, 26, 8743-8750.	1.6	113
22	Unraveling the Energetics and Dynamics of Ibuprofen in Mesoporous Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2009, 113, 18287-18291.	1.5	97
23	A Highly Hydrophobic Metal-Organic Framework Zn(BDC)(TED) _{0.5} for Adsorption and Separation of CH ₃ OH/H ₂ O and CO ₂ /CH ₄ : An Integrated Experimental and Simulation Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 6602-6609.	1.5	94
24	Metal-Organic Framework-Coated Optical Fibers as Light-Triggered Drug Delivery Vehicles. <i>Advanced Functional Materials</i> , 2016, 26, 3244-3249.	7.8	88
25	CUB-5: A Contoured Aliphatic Pore Environment in a Cubic Framework with Potential for Benzene Separation Applications. <i>Journal of the American Chemical Society</i> , 2019, 141, 3828-3832.	6.6	87
26	Facile stabilization of cyclodextrin metal-organic frameworks under aqueous conditions via the incorporation of C ₆₀ in their matrices. <i>Chemical Communications</i> , 2016, 52, 5973-5976.	2.2	81
27	Harnessing Lewis acidic open metal sites of metal-organic frameworks: the foremost route to achieve highly selective benzene sorption over cyclohexane. <i>Chemical Communications</i> , 2016, 52, 8215-8218.	2.2	76
28	Advances in adsorptive separation of benzene and cyclohexane by metal-organic framework adsorbents. <i>Coordination Chemistry Reviews</i> , 2021, 437, 213852.	9.5	74
29	Highly Porous Ionic rht Metal-Organic Framework for H ₂ and CO ₂ Storage and Separation: A Molecular Simulation Study. <i>Langmuir</i> , 2010, 26, 11196-11203.	1.6	72
30	Microwave-Assisted Solvothermal Synthesis and Optical Properties of Tagged MIL-140A Metal-Organic Frameworks. <i>Inorganic Chemistry</i> , 2013, 52, 12878-12880.	1.9	72
31	Upgrade of natural gas in rho zeolite-like metal-organic framework and effect of water: a computational study. <i>Energy and Environmental Science</i> , 2009, 2, 1088.	15.6	67
32	Enhancing selective CO ₂ adsorption via chemical reduction of a redox-active metal-organic framework. <i>Dalton Transactions</i> , 2013, 42, 9831.	1.6	64
33	Porous crystalline frameworks for thermocatalytic CO ₂ reduction: an emerging paradigm. <i>Energy and Environmental Science</i> , 2021, 14, 320-352.	15.6	61
34	Does functionalisation enhance CO ₂ uptake in interpenetrated MOFs? An examination of the IRMOF-9 series. <i>Chemical Communications</i> , 2014, 50, 3238-3241.	2.2	57
35	CO ₂ Adsorption in Azobenzene Functionalized Stimuli Responsive Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2016, 120, 16658-16667.	1.5	53
36	CO ₂ adsorption and separation in covalent organic frameworks with interlayer slipping. <i>CrystEngComm</i> , 2017, 19, 6950-6963.	1.3	51

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37	Gas Adsorption and Separation by the Al-Based Metal-Organic Framework MIL-160. <i>Journal of Physical Chemistry C</i> , 2017, 121, 26822-26832.	1.5	51
38	A Water-Stable Cationic Metal-Organic Framework with Hydrophobic Pore Surfaces as an Efficient Scavenger of Oxo-Anion Pollutants from Water. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 41810-41818.	4.0	51
39	Enhancing Multicomponent Metal-Organic Frameworks for Low Pressure Liquid Organic Hydrogen Carrier Separations. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 6090-6098.	7.2	50
40	Molecular Insight into Adsorption and Diffusion of Alkane Isomer Mixtures in Metal-Organic Frameworks. <i>Journal of Physical Chemistry B</i> , 2009, 113, 9129-9136.	1.2	48
41	Nitrogen-Doped Mesoporous Carbon for Carbon Capture – A Molecular Simulation Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 7106-7110.	1.5	48
42	Effect of Pore Topology and Accessibility on Gas Adsorption Capacity in Zeolitic Imidazolate Frameworks: Bringing Molecular Simulation Close to Experiment. <i>Journal of Physical Chemistry C</i> , 2011, 115, 8126-8135.	1.5	47
43	Tuning the cavities of zirconium-based MIL-140 frameworks to modulate CO ₂ adsorption. <i>Chemical Communications</i> , 2015, 51, 11286-11289.	2.2	47
44	Cation Characterization and CO ₂ Capture in Li ⁺ -Exchanged Metal-Organic Frameworks: From First-Principles Modeling to Molecular Simulation. <i>Industrial & Engineering Chemistry Research</i> , 2011, 50, 62-68.	1.8	43
45	Metal-Organic Framework-Enhanced Solid-Phase Microextraction Mass Spectrometry for the Direct and Rapid Detection of Perfluorooctanoic Acid in Environmental Water Samples. <i>Analytical Chemistry</i> , 2020, 92, 6900-6908.	3.2	41
46	High Alkaline Water-Splitting Activity of Mesoporous 3D Heterostructures: An Amorphous-Shell@Crystalline-Core Nano-Assembly of Co-Ni-Phosphate Ultrathin Nanosheets and Doped Cobalt Nitride Nanowires. <i>Advanced Science</i> , 2022, 9, .	4.0	41
47	Hysteretic carbon dioxide sorption in a novel copper(ii)-indazole-carboxylate porous coordination polymer. <i>Chemical Communications</i> , 2012, 48, 11558.	2.2	39
48	Rapid, selective capture of toxic oxo-anions of Se(^{iv}), Se(^{vi}) and As(^v) from water by an ionic metal-organic framework (iMOF). <i>Journal of Materials Chemistry A</i> , 2021, 9, 6499-6507.	5.2	39
49	Computer-Aided Design of Interpenetrated Tetrahydrofuran-Functionalized 3D Covalent Organic Frameworks for CO ₂ Capture. <i>Crystal Growth and Design</i> , 2012, 12, 5349-5356.	1.4	37
50	Methane Adsorption and Separation in Slipped and Functionalized Covalent Organic Frameworks. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 4767-4778.	1.8	36
51	Polar Pore Surface Guided Selective CO ₂ Adsorption in a Prefunctionalized Metal-Organic Framework. <i>Crystal Growth and Design</i> , 2017, 17, 3581-3587.	1.4	34
52	Exploiting stable radical states for multifunctional properties in triarylamine-based porous organic polymers. <i>Journal of Materials Chemistry A</i> , 2014, 2, 12466-12474.	5.2	33
53	Acoustomicrofluidic assembly of oriented and simultaneously activated metal-organic frameworks. <i>Nature Communications</i> , 2019, 10, 2282.	5.8	33
54	Three-in-One C ₂ H ₂ Selectivity-Guided Adsorptive Separation across an Isorecticular Family of Cationic Square Lattice MOFs. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	33

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55	On/off porosity switching and post-assembly modifications of Cu ₄ L ₄ metal-organic polyhedra. <i>Chemical Science</i> , 2020, 11, 3664-3671.	3.7	31
56	Prediction of O ₂ /N ₂ Selectivity in Metal-Organic Frameworks via High-Throughput Computational Screening and Machine Learning. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 736-749.	4.0	30
57	Atomistic Insight into Adsorption, Mobility, and Vibration of Water in Ion-Exchanged Zeolite-like Metal-Organic Frameworks. <i>ACS Nano</i> , 2009, 3, 2563-2572.	7.3	28
58	The first example of a zirconium-oxide based metal-organic framework constructed from monocarboxylate ligands. <i>Dalton Transactions</i> , 2015, 44, 1516-1519.	1.6	26
59	Stabilizing the Extrinsic Porosity in Metal-Organic Cages-Based Supramolecular Framework by In Situ Catalytic Polymerization. <i>CCS Chemistry</i> , 2021, 3, 1382-1390.	4.6	25
60	Reversing Benzene/Cyclohexane Selectivity through Varying Supramolecular Interactions Using Aliphatic, Isoreticular MOFs. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 30885-30890.	4.0	24
61	Postcombustion CO ₂ Capture in Functionalized Porous Coordination Networks. <i>Journal of Physical Chemistry C</i> , 2013, 117, 26976-26987.	1.5	21
62	A New Structural Family of Gas-Sorbing Coordination Polymers Derived from Phenolic Carboxylic Acids. <i>Chemistry - A European Journal</i> , 2015, 21, 18057-18061.	1.7	21
63	Plasmonic metal-organic framework nanocomposites enabled by degenerately doped molybdenum oxides. <i>Journal of Colloid and Interface Science</i> , 2021, 588, 305-314.	5.0	21
64	Multifunctional Behavior of Sulfonate-Based Hydrolytically Stable Microporous Metal-Organic Frameworks. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 39049-39055.	4.0	18
65	Porous Aromatic Frameworks Impregnated with Lithiated Fullerenes for Natural Gas Purification. <i>Journal of Physical Chemistry C</i> , 2015, 119, 9347-9354.	1.5	17
66	Hetero-metallic metal-organic frameworks for room-temperature NO ₂ sensing. <i>Journal of Colloid and Interface Science</i> , 2022, 610, 304-312.	5.0	15
67	Heterometallic Metal Organic Frameworks for Air Separation: A Computational Study. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 15718-15731.	1.8	14
68	Interpenetrated Zirconium-Organic Frameworks: Small Cavities versus Functionalization for CO ₂ Capture. <i>Journal of Physical Chemistry C</i> , 2016, 120, 13013-13023.	1.5	13
69	Porous Aromatic Frameworks Impregnated with Fullerenes for Enhanced Methanol/Water Separation. <i>Langmuir</i> , 2014, 30, 14621-14630.	1.6	12
70	Strategies toward Enhanced Low-Pressure Volumetric Hydrogen Storage in Nanoporous Cryoadsorbents. <i>Langmuir</i> , 2013, 29, 15689-15697.	1.6	11
71	Elucidating the mechanisms of Paraffin-Olefin separations using nanoporous adsorbents: An overview. <i>iScience</i> , 2021, 24, 103042.	1.9	11
72	Enhancing Multicomponent Metal-Organic Frameworks for Low Pressure Liquid Organic Hydrogen Carrier Separations. <i>Angewandte Chemie</i> , 2020, 132, 6146-6154.	1.6	10

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73	Systematic review on sono-assisted CO ₂ stripping, solvent recovery and energy demand aspects in solvent-based post-combustion carbon dioxide capture process. <i>Chemical Engineering and Processing: Process Intensification</i> , 2022, 170, 108723.	1.8	10
74	Aqueous contaminant detection via UiO-66 thin film optical fiber sensor platform with fast Fourier transform based spectrum analysis. <i>Journal Physics D: Applied Physics</i> , 2018, 51, 025601.	1.3	8
75	Computational materials chemistry for carbon capture using porous materials. <i>Journal Physics D: Applied Physics</i> , 2017, 50, 463002.	1.3	7
76	The Effect of Sterically Active Ligand Substituents on Gas Adsorption within a Family of 3D Zn-Based Coordination Polymers. <i>Inorganic Chemistry</i> , 2020, 59, 8871-8881.	1.9	7
77	Residual solvent induced physical morphology and gas permeation in polyamide-imide membrane: Experimental investigation and molecular simulations. <i>European Polymer Journal</i> , 2022, 165, 111012.	2.6	6
78	Computational design of multilayer frameworks to achieve DOE target for on-board methane delivery. <i>Carbon</i> , 2019, 152, 206-217.	5.4	5
79	A QCM-based ¹³ C NMR mechanistic study of gas adsorption by plasmid DNA and DNA@[Bmim][PF6] construct. <i>RSC Advances</i> , 2016, 6, 81318-81329.	1.7	3
80	Molecular Computations of Adsorption in Nanoporous Materials. , 2010, , 69-100.		2
81	Corresponding States Theory for the Freezing of Ionic Liquids. <i>Industrial & Engineering Chemistry Research</i> , 2011, 50, 234-238.	1.8	2
82	Mixed donor, phenanthroline photoactive MOFs with favourable CO ₂ selectivity. <i>Chemical Communications</i> , 2020, 56, 13377-13380.	2.2	2
83	Three-Coordinate C ₂ H ₂ Selectivity-Guided Adsorptive Separation across an Isoreticular Family of Cationic Square-Lattice MOFs. <i>Angewandte Chemie</i> , 2022, 134, e202114132.	1.6	2
84	Lattice response of the porous coordination framework Zn(hba) to guest adsorption. <i>Powder Diffraction</i> , 2017, 32, S49-S53.	0.4	1
85	Tunable CO ₂ binding enthalpies by redox modulation of an electroactive MOF-74 framework. <i>Materials Advances</i> , 2021, 2, 2112-2119.	2.6	1