Tina Duren

List of Publications by Year
in descending order

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63	5,704	126858	123376
papers	citations	33 h-index	61 g-index

65	65	65	5807
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Design of New Materials for Methane Storage. Langmuir, 2004, 20, 2683-2689.	1.6	663
2	Using molecular simulation to characterise metalâ€“organic frameworks for adsorption applications. Chemical Society Reviews, 2009, 38, 1237.	18.7	613
3	Effects of Surface Area, Free Volume, and Heat of Adsorption on Hydrogen Uptake in Metalâˆ’Organic Frameworks. Journal of Physical Chemistry B, 2006, 110, 9565-9570.	1.2	558
4	Calculating Geometric Surface Areas as a Characterization Tool for Metalâˆ’Organic Frameworks. Journal of Physical Chemistry C, 2007, 111, 15350-15356.	1.5	498
5	Synthesis of MIL-102, a Chromium Carboxylate Metalâˆ’Organic Framework, with Gas Sorption Analysis. Journal of the American Chemical Society, 2006, 128, 14889-14896.	6.6	229
6	Flexibility and swing effect on the adsorption of energy-related gases on ZIF-8: combined experimental and simulation study. Dalton Transactions, 2012, 41, 10752.	1.6	176
7	Elucidating the Breathing of the Metalâ€“Organic Framework MIL-53(Sc) with ab Initio Molecular Dynamics Simulations and in Situ X-ray Powder Diffraction Experiments. Journal of the American Chemical Society, 2013, 135, 15763-15773.	6.6	173
8	Assessment of Isoreticular Metalâˆ’Organic Frameworks for Adsorption Separations:Â A Molecular Simulation Study of Methane/n-Butane Mixtures. Journal of Physical Chemistry B, 2004, 108, 15703-15708.	1.2	165
9	p-Xylene-Selective Metalâ€“Organic Frameworks: A Case of Topology-Directed Selectivity. Journal of the American Chemical Society, 2011, 133, 18526-18529.	6.6	159
10	Understanding the adsorption process in ZIF-8 using high pressure crystallography and computational modelling. Nature Communications, 2018, 9, 1429.	5.8	146
11	Adsorption of Methane, Ethane, and Their Binary Mixtures on MCM-41:Â Experimental Evaluation of Methods for the Prediction of Adsorption Equilibrium. Langmuir, 2002, 18, 2693-2701.	1.6	141
12	Protecting group and switchable pore-discriminating adsorption properties of a hydrophilicâ€“hydrophobic metalâ€“organic framework. Nature Chemistry, 2011, 3, 304-310.	6.6	141
13	Methane storage mechanism in the metal-organic framework Cu3(btc)2: An in situ neutron diffraction study. Microporous and Mesoporous Materials, 2010, 136, 50-58.	2.2	132
14	Molecular modelling of adsorption in novel nanoporous metalâ€“organic materials. Molecular Physics, 2004, 102, 211-221.	0.8	126
15	Interdependent lateral interactions, hydrophobicity and acid strength and their influence on the catalytic activity of nanoporous sulfonic acid silicas. Green Chemistry, 2010, 12, 1383.	4.6	109
16	A Computational and Experimental Approach Linking Disorder, Highâ€Pressure Behavior, and Mechanical Properties in UiO Frameworks. Angewandte Chemie - International Edition, 2016, 55, 2401-2405.	7.2	103
17	Improving Predictions of Gas Adsorption in Metalâ€“Organic Frameworks with Coordinatively Unsaturated Metal Sites: Model Potentials, ab initio Parameterization, and GCMC Simulations. Journal of Physical Chemistry C, 2012, 116, 18899-18909.	1.5	102
18	A novel structural form of MIL-53 observed for the scandium analogue and its response to temperature variation and CO₂adsorption. Dalton Transactions, 2012, 41, 3937-3941.	1.6	95

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19	Evaluation of Ideal Adsorbed Solution Theory as a Tool for the Design of Metalâ€“Organic Framework Materials. Industrial & Engineering Chemistry Research, 2012, 51, 4911-4921.	1.8	94
20	Accurate Prediction of Methane Adsorption in a Metalâ€“Organic Framework with Unsaturated Metal Sites by Direct Implementation of an ab Initio Derived Potential Energy Surface in GCMC Simulation. Journal of Physical Chemistry C, 2011, 115, 23074-23080.	1.5	86
21	Tuning the Mechanical Response of Metalâ€“Organic Frameworks by Defect Engineering. Journal of the American Chemical Society, 2018, 140, 11581-11584.	6.6	82
22	Structural Chemistry, Monoclinic-to-Orthorhombic Phase Transition, and CO₂ Adsorption Behavior of the Small Pore Scandium Terephthalate, Sc₂(O₂CC₆H₄CO₂)₃, and Its Nitro- And Amino-Functionalized Derivatives. Inorganic Chemistry, 2011, 50, 10844-10858.	1.9	75
23	Syntheses, structures and properties of cadmium benzenedicarboxylate metalâ€“organic frameworks. Dalton Transactions, 2008, , 2465.	1.6	63
24	A Multiscale Study of MOFs as Adsorbents in H₂ PSA Purification. Industrial & Engineering Chemistry Research, 2013, 52, 9946-9957.	1.8	63
25	Stabilization of Scandium Terephthalate MOFs against Reversible Amorphization and Structural Phase Transition by Guest Uptake at Extreme Pressure. Journal of the American Chemical Society, 2014, 136, 8606-8613.	6.6	63
26	Multirate delivery of multiple therapeutic agents from metal-organic frameworks. APL Materials, 2014, 2, .	2.2	58
27	Tuning the Swing Effect by Chemical Functionalization of Zeolitic Imidazolate Frameworks. Journal of the American Chemical Society, 2018, 140, 382-387.	6.6	55
28	Unusual Adsorption Behavior on Metalâ˜Organic Frameworks. Langmuir, 2010, 26, 14694-14699.	1.6	52
29	Polymorphism of metalâ€“organic frameworks: direct comparison of structures and theoretical N₂-uptake of topological pto- and tbo-isomers. Chemical Communications, 2014, 50, 4207-4210.	2.2	45
30	Calix[4]arene-based metalâ€“organic frameworks: towards hierarchically porous materials. Chemical Communications, 2012, 48, 4824.	2.2	40
31	Ultra-large supramolecular coordination cages composed of endohedral Archimedean and Platonic bodies. Nature Communications, 2017, 8, 15268.	5.8	39
32	Conformational isomerism controls collective flexibility in metalâ€“organic framework DUT-8(Ni). Physical Chemistry Chemical Physics, 2019, 21, 674-680.	1.3	39
33	Molecular simulation of adsorption and transport diffusion of model fluids in carbon nanotubes. Molecular Physics, 2002, 100, 3741-3751.	0.8	38
34	Experiences with the publicly available multipurpose simulation code, Music. Molecular Simulation, 2013, 39, 1223-1232.	0.9	33
35	Study of molecular shape and non-ideality effects on mixture adsorption isotherms of small molecules in carbon nanotubes: A grand canonical Monte Carlo simulation study. Chemical Engineering Science, 2002, 57, 2439-2448.	1.9	31
36	Triphasic Nature of Polymers of Intrinsic Microporosity Induces Storage and Catalysis Effects in Hydrogen and Oxygen Reactivity at Electrode Surfaces. ChemElectroChem, 2019, 6, 252-259.	1.7	30

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37	Composition dependent transport diffusion coefficients of CH4/CF4 mixtures in carbon nanotubes by non-equilibrium molecular dynamics simulations. Chemical Engineering Science, 2002, 57, 1343-1354.	1.9	28
38	Understanding the Kinetic and Thermodynamic Origins of Xylene Separation in UiO-66(Zr) via Molecular Simulation. Journal of Physical Chemistry C, 2016, 120, 18651-18658.	1.5	28
39	Effect of Surface Group Functionalization on the CO₂/N₂ Separation Properties of MCM-41: A Grand-Canonical Monte Carlo Simulation Study. Journal of Physical Chemistry C, 2010, 114, 18538-18547.	1.5	27
40	Origin of Enantioselectivity in a Chiral Metalâ€“Organic Framework: A Molecular Simulation Study. Journal of Physical Chemistry C, 2012, 116, 20874-20881.	1.5	27
41	A Computational and Experimental Approach Linking Disorder, Highâ€Pressure Behavior, and Mechanical Properties in UiO Frameworks. Angewandte Chemie, 2016, 128, 2447-2451.	1.6	24
42	Grand canonical molecular dynamics simulations of transport diffusion in geometrically heterogeneous pores. Physical Chemistry Chemical Physics, 2003, 5, 369-375.	1.3	23
43	Modulatorâ€Controlled Synthesis of Microporous STAâ€26, an Interpenetrated 8,3â€Connected Zirconium MOF with the theâ€i Topology, and its Reversible Lattice Shift. Chemistry - A European Journal, 2018, 24, 6115-6126.	1.7	23
44	STA-27, a porous Lewis acidic scandium MOF with an unexpected topology type prepared with 2,3,5,6-tetrakis(4-carboxyphenyl)pyrazine. Journal of Materials Chemistry A, 2019, 7, 5685-5701.	5.2	22
45	Hydrogen Uptake by {H[Mg(HCOO)₃]âŠƒNHMe₂}_{âˆž} and Determination of Its H₂ Adsorption Sites through Monte Carlo Simulations. Langmuir, 2011, 27, 10124-10131.	1.6	21
46	The synthesis, structures and reactions of zinc and cobalt metalâ€“organic frameworks incorporating an alkyne-based dicarboxylate linker. CrystEngComm, 2012, 14, 188-192.	1.3	20
47	Influence of Surface Groups on the Diffusion of Gases in MCM-41: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2011, 115, 10651-10660.	1.5	19
48	Metalâ€“Organic Frameworks from Divalent Metals and 1,4-Benzenedicarboxylate with Bidentate Pyridine-N-oxide Co-ligands. Crystal Growth and Design, 2015, 15, 891-899.	1.4	19
49	Heteroâ€Epitaxial Approach by Using Labile Coordination Sites to Prepare Catenated Metalâ€“Organic Frameworks with High Surface Areas. Chemistry - A European Journal, 2014, 20, 3595-3599.	1.7	16
50	Role of particle size and surface functionalisation on the flexibility behaviour of switchable metalâ€“organic framework DUT-8(Ni). Journal of Materials Chemistry A, 2020, 8, 22703-22711.	5.2	14
51	Framework Isomerism: Highly Augmented Copper(II)â€Paddlewheelâ€ÂBased MOF with Unusual (3,4)â€Net Topology. European Journal of Inorganic Chemistry, 2016, 2016, 1939-1943.	1.0	11
52	Pore-Network Connectivity and Molecular Sieving of Normal and Isoalkanes in the Mesoporous Silica SBA-2. Journal of Physical Chemistry C, 2014, 118, 10183-10190.	1.5	10
53	Inclusion and release of ant alarm pheromones from metalâ€“organic frameworks. Dalton Transactions, 2020, 49, 10334-10338.	1.6	10
54	Predicting Neopentane Isosteric Enthalpy of Adsorption at Zero Coverage in MCM-41. Langmuir, 2011, 27, 6738-6743.	1.6	8

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55	Hydrogen thermal desorption spectra: insights from molecular simulation. Dalton Transactions, 2012, 41, 3974.	1.6	8
56	Early stages of phase selection in MOF formation observed in molecular Monte Carlo simulations. RSC Advances, 2019, 9, 14382-14390.	1.7	8
57	Kinetic Monte Carlo Simulation of the Synthesis of Periodic Mesoporous Silicas SBA-2 and STAC-1: Generation of Realistic Atomistic Models. Journal of Physical Chemistry C, 2012, 116, 20966-20974.	1.5	7
58	Cisplatin uptake and release in pH sensitive zeolitic imidazole frameworks. Journal of Chemical Physics, 2021, 154, 244703.	1.2	7
59	How does the pore morphology influence the adsorption performance of metal-organic frameworks? A molecular simulation study of methane and ethane adsorption in Zn-MOFs. Studies in Surface Science and Catalysis, 2007, 170, 2042-2047.	1.5	3
60	Grand-Canonical Monte Carlo Adsorption Studies on SBA-2 Periodic Mesoporous Silicas. Journal of Physical Chemistry C, 2014, 118, 25441-25446.	1.5	3
61	Using molecular simulation to characterise metal-organic frameworks and judge their performance as adsorbents. Studies in Surface Science and Catalysis, 2007, , 161-168.	1.5	2
62	Molecular simulation of framework materials. Molecular Simulation, 2015, 41, 1309-1310.	0.9	0
63	Combined Experimental and Computational Study of Polycyclic Aromatic Compound Aggregation: The Impact of Solvent Composition. Polycyclic Aromatic Compounds, 2023, 43, 3790-3809.	1.4	0