Tina Duren

List of Publications by Year
in descending order

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Version: 2024-02-01

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	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
2	Cisplatin uptake and release in pH sensitive zeolitic imidazole frameworks. Journal of Chemical Physics, 2021, 154, 244703.	1.2	7
3	Inclusion and release of ant alarm pheromones from metalâ€“organic frameworks. Dalton Transactions, 2020, 49, 10334-10338.	1.6	10
4	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
5	Conformational isomerism controls collective flexibility in metalâ€“organic framework DUT-8(Ni). Physical Chemistry Chemical Physics, 2019, 21, 674-680.	1.3	39
6	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
7	Early stages of phase selection in MOF formation observed in molecular Monte Carlo simulations. RSC Advances, 2019, 9, 14382-14390.	1.7	8
8	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
9	Understanding the adsorption process in ZIF-8 using high pressure crystallography and computational modelling. Nature Communications, 2018, 9, 1429.	5.8	146
10	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
11	Tuning the Swing Effect by Chemical Functionalization of Zeolitic Imidazolate Frameworks. Journal of the American Chemical Society, 2018, 140, 382-387.	6.6	55
12	Tuning the Mechanical Response of Metalâ€“Organic Frameworks by Defect Engineering. Journal of the American Chemical Society, 2018, 140, 11581-11584.	6.6	82
13	Ultra-large supramolecular coordination cages composed of endohedral Archimedean and Platonic bodies. Nature Communications, 2017, 8, 15268.	5.8	39
14	Framework Isomerism: Highly Augmented Copper(II)â€Paddlewheelâ€ABased MOF with Unusual (3,4)â€Net Topology. European Journal of Inorganic Chemistry, 2016, 2016, 1939-1943.	1.0	11
15	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
16	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
17	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
18	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

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19	Molecular simulation of framework materials. Molecular Simulation, 2015, 41, 1309-1310.	0.9	0
20	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
21	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
22	Grand-Canonical Monte Carlo Adsorption Studies on SBA-2 Periodic Mesoporous Silicas. Journal of Physical Chemistry C, 2014, 118, 25441-25446.	1.5	3
23	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
24	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
25	Multirate delivery of multiple therapeutic agents from metal-organic frameworks. APL Materials, 2014, 2, .	2.2	58
26	Experiences with the publicly available multipurpose simulation code, Music. Molecular Simulation, 2013, 39, 1223-1232.	0.9	33
27	A Multiscale Study of MOFs as Adsorbents in H₂ PSA Purification. Industrial & Engineering Chemistry Research, 2013, 52, 9946-9957.	1.8	63
28	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
29	Hydrogen thermal desorption spectra: insights from molecular simulation. Dalton Transactions, 2012, 41, 3974.	1.6	8
30	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
31	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
32	Calix[4]arene-based metalâ€“organic frameworks: towards hierarchically porous materials. Chemical Communications, 2012, 48, 4824.	2.2	40
33	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
34	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
35	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
36	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

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37	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
38	Predicting Neopentane Isosteric Enthalpy of Adsorption at Zero Coverage in MCM-41. Langmuir, 2011, 27, 6738-6743.	1.6	8
39	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
40	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
41	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
42	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
43	Protecting group and switchable pore-discriminating adsorption properties of a hydrophilicâ€“hydrophobic metalâ€“organic framework. Nature Chemistry, 2011, 3, 304-310.	6.6	141
44	Hydrogen Uptake by {H[Mg(HCOO)₃]âŠƒNHMe₂}_{â^ž} and Determination of Its H₂ Adsorption Sites through Monte Carlo Simulations. Langmuir, 2011, 27, 10124-10131.	1.6	21
45	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
46	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
47	Unusual Adsorption Behavior on Metalâ^'Organic Frameworks. Langmuir, 2010, 26, 14694-14699.	1.6	52
48	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
49	Using molecular simulation to characterise metalâ€“organic frameworks for adsorption applications. Chemical Society Reviews, 2009, 38, 1237.	18.7	613
50	Syntheses, structures and properties of cadmium benzenedicarboxylate metalâ€“organic frameworks. Dalton Transactions, 2008, , 2465.	1.6	63
51	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
52	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
53	Calculating Geometric Surface Areas as a Characterization Tool for Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2007, 111, 15350-15356.	1.5	498
54	Synthesis of MIL-102, a Chromium Carboxylate Metalâ^'Organic Framework, with Gas Sorption Analysis. Journal of the American Chemical Society, 2006, 128, 14889-14896.	6.6	229

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55	Effects of Surface Area, Free Volume, and Heat of Adsorption on Hydrogen Uptake in Metalâ˜Organic Frameworks. Journal of Physical Chemistry B, 2006, 110, 9565-9570.	1.2	558
56	Molecular modelling of adsorption in novel nanoporous metalâ€“organic materials. Molecular Physics, 2004, 102, 211-221.	0.8	126
57	Assessment of Isoreticular Metalâ˜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
58	Design of New Materials for Methane Storage. Langmuir, 2004, 20, 2683-2689.	1.6	663
59	Grand canonical molecular dynamics simulations of transport diffusion in geometrically heterogeneous pores. Physical Chemistry Chemical Physics, 2003, 5, 369-375.	1.3	23
60	Molecular simulation of adsorption and transport diffusion of model fluids in carbon nanotubes. Molecular Physics, 2002, 100, 3741-3751.	0.8	38
61	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
62	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
63	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