A Ozgur Yazaydin

List of Publications by Year
in descending order

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66 papers	10,389 citations	126708 33 h-index	106150 65 g-index
77 all docs	77 docs citations	77 times ranked	11484 citing authors

#	Article	IF	Citations
1	Coordinationâ€Induced Band Gap Reduction in a Metalâ€“Organic Framework. Chemistry - A European Journal, 2022, 28, e202104041.	1.7	4
2	Tuning the Transport Properties of Gases in Porous Graphene Membranes with Controlled Pore Size and Thickness. Advanced Materials, 2022, 34, e2106785.	11.1	18
3	1-Bromopropane Capture with Hydrophobic Zeolites: Force Field Development and Molecular Simulations. Journal of Physical Chemistry C, 2022, 126, 5728-5734.	1.5	1
4	Electrically Conductive Photoluminescent Porphyrin Phosphonate Metalâ€“Organic Frameworks. Advanced Optical Materials, 2022, 10, .	3.6	8
5	Supercritical carbon dioxide enhanced natural gas recovery from kerogen micropores. Journal of CO2 Utilization, 2022, 62, 102105.	3.3	5
6	The role of hydrogen bonding in the dehydration of bioalcohols in hydrophobic pervaporation membranes. Journal of Molecular Liquids, 2021, 340, 117297.	2.3	5
7	ZnO@ZIF-8: Gas sensitive core-shell hetero-structures show reduced cross-sensitivity to humidity. Sensors and Actuators B: Chemical, 2020, 304, 127184.	4.0	34
8	Modeling of Gas Transport through Polymer/MOF Interfaces: A Microsecond-Scale Concentration Gradient-Driven Molecular Dynamics Study. Chemistry of Materials, 2020, 32, 1288-1296.	3.2	64
9	Rapid and Efficient Removal of Perfluorooctanoic Acid from Water with Fluorine-Rich Calixarene-Based Porous Polymers. ACS Applied Materials & Interfaces, 2020, 12, 43160-43166.	4.0	40
10	Does Confinement Enable Methane Hydrate Growth at Low Pressures? Insights from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2020, 124, 11015-11022.	1.5	31
11	Semiconductive microporous hydrogen-bonded organophosphonic acid frameworks. Nature Communications, 2020, 11, 3180.	5.8	50
12	A Nanotubular Metalâ€“Organic Framework with a Narrow Bandgap from Extended Conjugation**. Chemistry - A European Journal, 2020, 26, 14813-14816.	1.7	18
13	Role of Cations in the Methane/Carbon Dioxide Partitioning in Nano- and Mesopores of Illite Using Constant Reservoir Composition Molecular Dynamics Simulation. Journal of Physical Chemistry C, 2020, 124, 2490-2500.	1.5	20
14	Direct Simulation of Ternary Mixture Separation in a ZIFâ€8 Membrane at Molecular Scale. Advanced Theory and Simulations, 2019, 2, 1900120.	1.3	10
15	A cobalt arylphosphonate MOF â€“ superior stability, sorption and magnetism. Chemical Communications, 2019, 55, 3053-3056.	2.2	50
16	Gas permeation through single-crystal ZIF-8 membranes. Journal of Membrane Science, 2019, 575, 209-216.	4.1	61
17	Alkali Phosphonate Metalâ€“Organic Frameworks. Chemistry - A European Journal, 2019, 25, 11214-11217.	1.7	20
18	Understanding methane/carbon dioxide partitioning in clay nano- and meso-pores with constant reservoir composition molecular dynamics modeling. Physical Chemistry Chemical Physics, 2019, 21, 6917-6924.	1.3	21

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19	Tuning the Hydrophobicity of Layer-Structure Silicates To Promote Adsorption of Nonaqueous Fluids: Effects of F^{â€“} for OH^{â€“} Substitution on CO₂ Partitioning into Smectite Interlayers. Journal of Physical Chemistry C, 2019, 123, 4848-4855.	1.5	15
20	Clay Swelling in Dry Supercritical Carbon Dioxide: Effects of Interlayer Cations on the Structure, Dynamics, and Energetics of CO₂ Intercalation Probed by XRD, NMR, and GCMD Simulations. Journal of Physical Chemistry C, 2018, 122, 4391-4402.	1.5	42
21	Adsorption of Atrazine from Water in Metalâ€“Organic Framework Materials. Journal of Chemical & Engineering Data, 2018, 63, 2368-2375.	1.0	71
22	Electric field induced rotation of halogenated organic linkers in isoreticular metalâ€“organic frameworks for nanofluidic applications. Molecular Systems Design and Engineering, 2018, 3, 951-958.	1.7	16
23	Competitive Adsorption of H₂O and CO₂ in 2-Dimensional Nanoconfinement: GCMD Simulations of Cs- and Ca-Hectorites. Journal of Physical Chemistry C, 2018, 122, 23460-23469.	1.5	17
24	From 2-methylimidazole to 1,2,3-triazole: a topological transformation of ZIF-8 and ZIF-67 by post-synthetic modification. Chemical Communications, 2017, 53, 2028-2031.	2.2	61
25	Design of electric field controlled molecular gates mounted on metalâ€“organic frameworks. Journal of Materials Chemistry A, 2017, 5, 8690-8696.	5.2	51
26	From Tetrahedral Tetraphosphonic Acids E[p -C₆ H₄ P(O)(OH)₂]₄ (E=C, Si) to Porous Cu- and Zn-MOFs with Large Surface Areas. ChemistrySelect, 2017, 2, 3035-3038.	0.7	19
27	Concentration gradient driven molecular dynamics: a new method for simulations of membrane permeation and separation. Chemical Science, 2017, 8, 3858-3865.	3.7	66
28	Tipping Point for Expansion of Layered Aluminosilicates in Weakly Polar Solvents: Supercritical CO₂. ACS Applied Materials & Interfaces, 2017, 9, 36783-36791.	4.0	38
29	Molecular Dynamics Study of CO₂ and H₂O Intercalation in Smectite Clays: Effect of Temperature and Pressure on Interlayer Structure and Dynamics in Hectorite. Journal of Physical Chemistry C, 2017, 121, 24527-24540.	1.5	34
30	Short Naphthalene Organophosphonate Linkers to Microporous Frameworks. ChemistrySelect, 2017, 2, 7050-7053.	0.7	8
31	Rapid and Efficient Removal of Carbamazepine from Water by UiO-67. Industrial & Engineering Chemistry Research, 2017, 56, 15122-15130.	1.8	51
32	Molecular simulation studies of hydrogen enriched methane (HEM) storage in Covalent Organic Frameworks. Microporous and Mesoporous Materials, 2016, 231, 138-146.	2.2	7
33	Structure, Energetics, and Dynamics of Cs⁺ and H₂O in Hectorite: Molecular Dynamics Simulations with an Unconstrained Substrate Surface. Journal of Physical Chemistry C, 2016, 120, 10298-10310.	1.5	60
34	Water Structure and Dynamics in Smectites: X-ray Diffraction and ²H NMR Spectroscopy of Mgâ€“, Caâ€“, Srâ€“, Naâ€“, Csâ€“, and Pbâ€“Hectorite. Journal of Physical Chemistry C, 2016, 120, 8863-8876.	1.5	32
35	Anhydrous proton conducting poly(vinyl alcohol) (PVA)/ poly(2-acrylamido-2-methylpropane sulfonic) Tj ETQq1 1 0.784314 rgBT /Ove 11321-11330.	3.8	28
36	Cation and Water Structure, Dynamics, and Energetics in Smectite Clays: A Molecular Dynamics Study of Caâ€“Hectorite. Journal of Physical Chemistry C, 2016, 120, 12429-12439.	1.5	48

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37	Screening of Zeolitic Imidazolate Frameworks for Preconcentration of Hazardous Chemicals. NATO Science for Peace and Security Series A: Chemistry and Biology, 2015, , 177-189.	0.5	0
38	NMR and computational molecular modeling studies of mineral surfaces and interlayer galleries: A review. American Mineralogist, 2015, 100, 1341-1354.	0.9	32
39	Molecular dynamics modeling of carbon dioxide, water and natural organic matter in Na-hectorite. Physical Chemistry Chemical Physics, 2015, 17, 23356-23367.	1.3	20
40	Selective Gas Adsorption in a Pair of Robust Isostructural MOFs Differing in Framework Charge and Anion Loading. Inorganic Chemistry, 2014, 53, 12076-12083.	1.9	29
41	A combined experimental and quantum chemical study of CO2 adsorption in the metalâ€“organic framework CPO-27 with different metals. Chemical Science, 2013, 4, 3544.	3.7	172
42	Hydrogen and methane storage in ultrahigh surface area Metalâ€“Organic Frameworks. Microporous and Mesoporous Materials, 2013, 182, 185-190.	2.2	36
43	The effect of SO2 on CO2 capture in zeolitic imidazolate frameworks. Physical Chemistry Chemical Physics, 2013, 15, 11856.	1.3	59
44	Structure, Energetics, and Dynamics of Smectite Clay Interlayer Hydration: Molecular Dynamics and Metadynamics Investigation of Na-Hectorite. Journal of Physical Chemistry C, 2013, 117, 5172-5187.	1.5	102
45	A comparative study of CO2, CH4 and N2 adsorption in ZIF-8, Zeolite-13X and BPL activated carbon. Chemical Physics, 2013, 412, 72-76.	0.9	263
46	Dehydration-Induced Amorphous Phases of Calcium Carbonate. Journal of Physical Chemistry B, 2013, 117, 3328-3336.	1.2	74
47	Synergistic Interaction of Paclitaxel and Curcumin with Cyclodextrin Polymer Complexation in Human Cancer Cells. Molecular Pharmaceutics, 2013, 10, 2676-2683.	2.3	97
48	Computerâ€Assisted Screening of Ordered Crystalline Nanoporous Adsorbents for Separation of Alkane Isomers. Angewandte Chemie - International Edition, 2012, 51, 11867-11871.	7.2	89
49	Structure and Transformation of Amorphous Calcium Carbonate: A Solid-State ⁴³Ca NMR and Computational Molecular Dynamics Investigation. Chemistry of Materials, 2012, 24, 1828-1836.	3.2	70
50	Metalâ€“Organic Framework Materials with Ultrahigh Surface Areas: Is the Sky the Limit?. Journal of the American Chemical Society, 2012, 134, 15016-15021.	6.6	1,497
51	How Well Do Metalâ€“Organic Frameworks Tolerate Flue Gas Impurities?. Journal of Physical Chemistry C, 2012, 116, 22987-22991.	1.5	60
52	Two Large-Pore Metalâ€“Organic Frameworks Derived from a Single Polytopic Strut. Crystal Growth and Design, 2012, 12, 1075-1080.	1.4	31
53	Screening CO₂/N₂ selectivity in metalâ€organic frameworks using Monte Carlo simulations and ideal adsorbed solution theory. Canadian Journal of Chemical Engineering, 2012, 90, 825-832.	0.9	46
54	De novo synthesis of a metalâ€“organic framework material featuring ultrahigh surface area and gas storage capacities. Nature Chemistry, 2010, 2, 944-948.	6.6	1,535

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55	Evaluation of the BET Method for Determining Surface Areas of MOFs and Zeolites that Contain Ultra-Micropores. Langmuir, 2010, 26, 5475-5483.	1.6	257
56	Ultrahigh Porosity in Metal-Organic Frameworks. Science, 2010, 329, 424-428.	6.0	3,306
57	Molecular simulation of water adsorption in silicalite: Effect of silanol groups and different cations. Microporous and Mesoporous Materials, 2009, 123, 169-176.	2.2	57
58	Screening of Metalâ˜Organic Frameworks for Carbon Dioxide Capture from Flue Gas Using a Combined Experimental and Modeling Approach. Journal of the American Chemical Society, 2009, 131, 18198-18199.	6.6	816
59	Enhanced CO₂ Adsorption in Metal-Organic Frameworks via Occupation of Open-Metal Sites by Coordinated Water Molecules. Chemistry of Materials, 2009, 21, 1425-1430.	3.2	523
60	Computing Adsorbate/Adsorbent Binding Energies and Henry's Law Constants from Molecular Simulations. Environmental Engineering Science, 2009, 26, 297-304.	0.8	5
61	A molecular simulation approach to the study of adsorption of hydrogen cyanide and methyl ethyl ketone in silicalite, mordenite and zeolite beta structures. Molecular Simulation, 2007, 33, 843-850.	0.9	11
62	Bubble point pressure estimates from Gibbs ensemble simulations. Fluid Phase Equilibria, 2007, 260, 195-198.	1.4	11
63	Simulating the vapourâ€“liquid equilibria of 1,4-dioxane. Molecular Simulation, 2006, 32, 657-662.	0.9	8
64	Molecular Simulation of the Adsorption of MTBE in Silicalite, Mordenite, and Zeolite Beta. Journal of Physical Chemistry B, 2006, 110, 14458-14462.	1.2	37
65	Scanning electron microscopic studies of porous carbon electrodes used in alkaline fuel cells. Chemical Engineering Communications, 2003, 190, 976-985.	1.5	1
66	Diffusion Behavior of Methane in 3D Kerogen Models. Energy & Fuels, 0, , .	2.5	10