A Ozgur Yazaydin

List of Publications by Year in Descending Order

66 papers	8,638 citations	29 h-index	77 g-index
77 ext. papers	9,507 ext. citations	6.4 avg, IF	5.89 L-index

#	Paper	IF	Citations
66	1-Bromopropane Capture with Hydrophobic Zeolites: Force Field Development and Molecular Simulations. *Journal of Physical Chemistry C*, **2022**, 126, 5728-5734	3.8	0
65	Coordination-induced band gap reduction in a metal-organic framework. *Chemistry - A European Journal*, **2021**, e202104041	4.8	
64	Tuning the Transport Properties of Gases in Porous Graphene Membranes with Controlled Pore Size and Thickness. *Advanced Materials*, **2021**, e2106785	24	2
63	The role of hydrogen bonding in the dehydration of bioalcohols in hydrophobic pervaporation membranes. *Journal of Molecular Liquids*, **2021**, 340, 117297	6	1
62	Does Confinement Enable Methane Hydrate Growth at Low Pressures? Insights from Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2020**, 124, 11015-11022	3.8	12
61	Semiconductive microporous hydrogen-bonded organophosphonic acid frameworks. *Nature Communications*, **2020**, 11, 3180	17.4	22
60	A Nanotubular Metal-Organic Framework with a Narrow Bandgap from Extended Conjugation*. *Chemistry - A European Journal*, **2020**, 26, 14813-14816	4.8	9
59	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	3.8	11
58	Modeling of Gas Transport through Polymer/MOF Interfaces: A Microsecond-Scale Concentration Gradient-Driven Molecular Dynamics Study. *Chemistry of Materials*, **2020**, 32, 1288-1296	9.6	29
57	Rapid and Efficient Removal of Perfluorooctanoic Acid from Water with Fluorine-Rich Calixarene-Based Porous Polymers. *ACS Applied Materials & Interfaces*, **2020**, 12, 43160-43166	9.5	17
56	ZnO@ZIF-8: Gas sensitive core-shell hetero-structures show reduced cross-sensitivity to humidity. *Sensors and Actuators B: Chemical*, **2020**, 304, 127184	8.5	18
55	A cobalt arylphosphonate MOF - superior stability, sorption and magnetism. *Chemical Communications*, **2019**, 55, 3053-3056	5.8	34
54	Gas permeation through single-crystal ZIF-8 membranes. *Journal of Membrane Science*, **2019**, 575, 209-216	7.6	30
53	Alkali Phosphonate Metal-Organic Frameworks. *Chemistry - A European Journal*, **2019**, 25, 11214-11217	4.8	10
52	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	3.6	15
51	Tuning the Hydrophobicity of Layer-Structure Silicates To Promote Adsorption of Nonaqueous Fluids: Effects of F for OH Substitution on CO2 Partitioning into Smectite Interlayers. *Journal of Physical Chemistry C*, **2019**, 123, 4848-4855	3.8	9
50	Direct Simulation of Ternary Mixture Separation in a ZIF-8 Membrane at Molecular Scale. *Advanced Theory and Simulations*, **2019**, 2, 1900120	3.5	7

49	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	3.8	30
48	Adsorption of Atrazine from Water in Metal□Organic Framework Materials. *Journal of Chemical & Engineering Data*, **2018**, 63, 2368-2375	2.8	44
47	Electric field induced rotation of halogenated organic linkers in isoreticular metal□organic frameworks for nanofluidic applications. *Molecular Systems Design and Engineering*, **2018**, 3, 951-958	4.6	10
46	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	3.8	12
45	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	5.8	37
44	Design of electric field controlled molecular gates mounted on metal□organic frameworks. *Journal of Materials Chemistry A*, **2017**, 5, 8690-8696	13	41
43	From Tetrahedral Tetraphosphonic Acids E[p-C6H4P(O)(OH)2]4 (E=C, Si) to Porous Cu- and Zn-MOFs with Large Surface Areas. *ChemistrySelect*, **2017**, 2, 3035-3038	1.8	16
42	Concentration gradient driven molecular dynamics: a new method for simulations of membrane permeation and separation. *Chemical Science*, **2017**, 8, 3858-3865	9.4	43
41	Tipping Point for Expansion of Layered Aluminosilicates in Weakly Polar Solvents: Supercritical CO. *ACS Applied Materials & Interfaces*, **2017**, 9, 36783-36791	9.5	29
40	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	3.8	26
39	Short Naphthalene Organophosphonate Linkers to Microporous Frameworks. *ChemistrySelect*, **2017**, 2, 7050-7053	1.8	6
38	Rapid and Efficient Removal of Carbamazepine from Water by UiO-67. *Industrial & Engineering Chemistry Research*, **2017**, 56, 15122-15130	3.9	34
37	Cation and Water Structure, Dynamics, and Energetics in Smectite Clays: A Molecular Dynamics Study of Ca□Hectorite. *Journal of Physical Chemistry C*, **2016**, 120, 12429-12439	3.8	40
36	Molecular simulation studies of hydrogen enriched methane (HEM) storage in Covalent Organic Frameworks. *Microporous and Mesoporous Materials*, **2016**, 231, 138-146	5.3	6
35	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	3.8	50
34	Water Structure and Dynamics in Smectites: X-ray Diffraction and 2H NMR Spectroscopy of Mg□ Ca□Sr□Na□Cs□and Pb□Hectorite. *Journal of Physical Chemistry C*, **2016**, 120, 8863-8876	3.8	28
33	Anhydrous proton conducting poly(vinyl alcohol) (PVA)/ poly(2-acrylamido-2-methylpropane sulfonic acid) (PAMPS)/1,2,4-triazole composite membrane. *International Journal of Hydrogen Energy*, **2016**, 41, 11321-11330	6.7	23
32	Review. NMR and computational molecular modeling studies of mineral surfaces and interlayer galleries: A review. *American Mineralogist*, **2015**, 100, 1341-1354	2.9	25

31	Molecular dynamics modeling of carbon dioxide, water and natural organic matter in Na-hectorite. *Physical Chemistry Chemical Physics*, **2015**, 17, 23356-67	3.6	15
30	Screening of Zeolitic Imidazolate Frameworks for Preconcentration of Hazardous Chemicals. *NATO Science for Peace and Security Series A: Chemistry and Biology*, **2015**, 177-189	0.1	
29	Selective gas adsorption in a pair of robust isostructural MOFs differing in framework charge and anion loading. *Inorganic Chemistry*, **2014**, 53, 12076-83	5.1	28
28	A combined experimental and quantum chemical study of CO2 adsorption in the metal□organic framework CPO-27 with different metals. *Chemical Science*, **2013**, 4, 3544	9.4	142
27	Hydrogen and methane storage in ultrahigh surface area Metal□Organic Frameworks. *Microporous and Mesoporous Materials*, **2013**, 182, 185-190	5.3	28
26	The effect of SO2 on CO2 capture in zeolitic imidazolate frameworks. *Physical Chemistry Chemical Physics*, **2013**, 15, 11856-61	3.6	51
25	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	3.8	85
24	A comparative study of CO2, CH4 and N2 adsorption in ZIF-8, Zeolite-13X and BPL activated carbon. *Chemical Physics*, **2013**, 412, 72-76	2.3	207
23	Nanotechnology for Carbon Dioxide Capture **2013**, 517-559		
22	Dehydration-induced amorphous phases of calcium carbonate. *Journal of Physical Chemistry B*, **2013**, 117, 3328-36	3.4	54
21	Synergistic interaction of paclitaxel and curcumin with cyclodextrin polymer complexation in human cancer cells. *Molecular Pharmaceutics*, **2013**, 10, 2676-83	5.6	72
20	Computer-assisted screening of ordered crystalline nanoporous adsorbents for separation of alkane isomers. *Angewandte Chemie - International Edition*, **2012**, 51, 11867-71	16.4	81
19	Structure and Transformation of Amorphous Calcium Carbonate: A Solid-State 43Ca NMR and Computational Molecular Dynamics Investigation. *Chemistry of Materials*, **2012**, 24, 1828-1836	9.6	62
18	Metal-organic framework materials with ultrahigh surface areas: is the sky the limit?. *Journal of the American Chemical Society*, **2012**, 134, 15016-21	16.4	1210
17	How Well Do Metal□Organic Frameworks Tolerate Flue Gas Impurities?. *Journal of Physical Chemistry C*, **2012**, 116, 22987-22991	3.8	51
16	Two Large-Pore Metal□Organic Frameworks Derived from a Single Polytopic Strut. *Crystal Growth and Design*, **2012**, 12, 1075-1080	3.5	31
15	Screening CO2/N2 selectivity in metal-organic frameworks using Monte Carlo simulations and ideal adsorbed solution theory. *Canadian Journal of Chemical Engineering*, **2012**, 90, 825-832	2.3	41
14	De novo synthesis of a metal-organic framework material featuring ultrahigh surface area and gas storage capacities. *Nature Chemistry*, **2010**, 2, 944-8	17.6	1350

13	Evaluation of the BET method for determining surface areas of MOFs and zeolites that contain ultra-micropores. *Langmuir*, **2010**, 26, 5475-83	4	193
12	Ultrahigh porosity in metal-organic frameworks. *Science*, **2010**, 329, 424-8	33.3	2869
11	Molecular simulation of water adsorption in silicalite: Effect of silanol groups and different cations. *Microporous and Mesoporous Materials*, **2009**, 123, 169-176	5.3	54
10	Screening of metal-organic frameworks for carbon dioxide capture from flue gas using a combined experimental and modeling approach. *Journal of the American Chemical Society*, **2009**, 131, 18198-9	16.4	737
9	Enhanced CO2 Adsorption in Metal-Organic Frameworks via Occupation of Open-Metal Sites by Coordinated Water Molecules. *Chemistry of Materials*, **2009**, 21, 1425-1430	9.6	472
8	Computing Adsorbate/Adsorbent Binding Energies and Henry□s Law Constants from Molecular Simulations. *Environmental Engineering Science*, **2009**, 26, 297-304	2	5
7	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	2	10
6	Bubble point pressure estimates from Gibbs ensemble simulations. *Fluid Phase Equilibria*, **2007**, 260, 195-198	2.5	11
5	Simulating the vapour□liquid equilibria of 1,4-dioxane. *Molecular Simulation*, **2006**, 32, 657-662	2	8
4	Molecular simulation of the adsorption of MTBE in silicalite, mordenite, and zeolite beta. *Journal of Physical Chemistry B*, **2006**, 110, 14458-62	3.4	31
3	Scanning electron microscopic studies of porous carbon electrodes used in alkaline fuel cells. *Chemical Engineering Communications*, **2003**, 190, 976-985	2.2	1
2	Nanotechnology for Carbon Dioxide Capture359-401		1
1	Electrically Conductive Photoluminescent Porphyrin Phosphonate Metal□Organic Frameworks. *Advanced Optical Materials*,2200213	8.1	1