M GÃ¶ktug Ahunbay

List of Publications by Year
in descending order

38 papers	1,310 citations	448610 19 h-index	388640 36 g-index
40 all docs	40 docs citations	40 times ranked	1893 citing authors

#	Article	IF	Citations
1	Desalination Potential of Aquaporin-Inspired Functionalization of Carbon Nanotubes: Bridging Between Simulation and Experiment. ACS Applied Materials & Interfaces, 2022, 14, 28174-28185.	4.0	13
2	CO2/CH4 mixed-gas separation in PIM-1 at high pressures: Bridging atomistic simulations with process modeling. Journal of Membrane Science, 2021, 640, 119838.	4.1	20
3	Can crosslinking improve both CO2 permeability and plasticization resistance in 6FDAâ€“pBAPS/DABA copolyimides?. Polymer, 2020, 205, 122789.	1.8	12
4	MXene Materials for Designing Advanced Separation Membranes. Advanced Materials, 2020, 32, e1906697.	11.1	295
5	Technical and economic feasibility of the concurrent desalination and boron removal (CDBR) process. Desalination, 2020, 486, 114474.	4.0	18
6	Interfacial analysis of mixed-matrix membranes under exposure to high-pressure CO2. Journal of Membrane Science, 2020, 607, 118147.	4.1	16
7	In Silico Screening of Green Plasticizers for Poly(vinyl chloride). Macromolecules, 2019, 52, 2421-2430.	2.2	16
8	An atomistic insight on CO2 plasticization resistance of thermally rearranged 6FDA-bisAPAF. Journal of Membrane Science, 2018, 556, 23-33.	4.1	19
9	Prediction of CO2-induced plasticization pressure in polyimides via atomistic simulations. Journal of Membrane Science, 2018, 547, 146-155.	4.1	40
10	Energy optimization of a multistage reverse osmosis process for seawater desalination. Desalination, 2018, 429, 1-11.	4.0	40
11	Novel co-polyimides containing pBAPS (bis [4-(4-aminophenoxy) phenyl] sulfone) for CO 2 separation. Separation and Purification Technology, 2017, 178, 90-104.	3.9	8
12	Highly CO₂ Selective Microporous Metal-Imidazolate Framework-Based Mixed Matrix Membranes. ACS Applied Materials & Interfaces, 2017, 9, 35936-35946.	4.0	14
13	A novel energy-efficient concurrent desalination and boron removal (CDBR) process. Desalination, 2017, 423, 79-94.	4.0	10
14	Adsorption of perfluorohexane in BAM-P109 type activated carbon via molecular simulation. Adsorption Science and Technology, 2016, 34, 79-92.	1.5	7
15	Propylene/propane plasticization in polyimide membranes. Journal of Membrane Science, 2016, 501, 179-190.	4.1	41
16	Sod -ZMOF/Matrimid Â® mixed matrix membranes for CO 2 separation. Journal of Membrane Science, 2015, 489, 81-89.	4.1	35
17	Solvation of a Cellulose Microfibril in Imidazolium Acetate Ionic Liquids: Effect of a Cosolvent. Journal of Physical Chemistry B, 2014, 118, 141211094045002.	1.2	39
18	Prediction of perfluorohexane adsorption in BCR-704 zeolite via molecular simulation. Fluid Phase Equilibria, 2014, 366, 152-158.	1.4	6

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19	Propane/propylene separation in ion-exchanged zeolite-like metal organic frameworks. Microporous and Mesoporous Materials, 2014, 198, 185-193.	2.2	14
20	CO₂/CH₄ Separation in Ion-Exchanged Zeolite-like Metal Organic Frameworks with Sodalite Topology (sod-ZMOFs). Journal of Physical Chemistry C, 2013, 117, 15647-15658.	1.5	19
21	Silverâ€“Sodium Ion Exchange Dynamics in LTA Zeolite Membranes. Journal of Physical Chemistry C, 2013, 117, 1663-1671.	1.5	24
22	Molecular Simulation of Fibronectin Adsorption onto Polyurethane Surfaces. Langmuir, 2012, 28, 12619-12628.	1.6	24
23	Investigation of CO2-induced plasticization in fluorinated polyimide membranes via molecular simulation. Journal of Membrane Science, 2012, 417-418, 217-227.	4.1	75
24	Adsorption of Methyl Tertiary Butyl Ether and Trichloroethylene in MFI-Type Zeolites. Journal of Physical Chemistry C, 2012, 116, 21836-21843.	1.5	25
25	Monte Carlo Simulation of Water Adsorption in Hydrophobic MFI Zeolites with Hydrophilic Sites. Langmuir, 2011, 27, 4986-4993.	1.6	53
26	Molecular Dynamics Simulation of Water Diffusion in MFI-Type Zeolites. Journal of Physical Chemistry B, 2009, 113, 8073-8079.	1.2	51
27	MTBE adsorption and diffusion in silicalite-1. Microporous and Mesoporous Materials, 2008, 115, 93-97.	2.2	15
28	Molecular simulation of adsorption and diffusion of chlorinated alkenes in ZSM-5 zeolites. Journal of Chemical Physics, 2007, 127, 044707.	1.2	3
29	Molecular simulation of the thermophysical properties of fluids: From understanding toward quantitative predictions. Journal of Molecular Liquids, 2007, 134, 71-89.	2.3	99
30	Prediction of thermodynamic properties of heavy hydrocarbons by Monte Carlo simulation. Fluid Phase Equilibria, 2005, 228-229, 311-319.	1.4	7
31	Extension of the anisotropic united atoms intermolecular potential to amines, amides and alkanols. Fluid Phase Equilibria, 2005, 236, 25-41.	1.4	45
32	Gas Permeation Through Zeolite Single Crystal Membranes. Adsorption, 2005, 11, 313-318.	1.4	3
33	Effect of Surface Resistances on the Diffusion of Binary Mixtures in the Silicalite Single Crystal Membrane. Journal of Physical Chemistry B, 2005, 109, 923-929.	1.2	19
34	Optimized Intermolecular Potential for Aromatic Hydrocarbons Based on Anisotropic United Atoms. III. Polyaromatic and Naphthenoaromatic Hydrocarbons. Journal of Physical Chemistry B, 2005, 109, 2970-2976.	1.2	48
35	Optimized Intermolecular Potential for Aromatic Hydrocarbons Based on Anisotropic United Atoms. 2. Alkylbenzenes and Styrene. Journal of Physical Chemistry B, 2004, 108, 14115-14123.	1.2	37
36	Prediction of thermodynamic properties of heavy hydrocarbons by Monte Carlo simulation. Fluid Phase Equilibria, 2004, 224, 73-81.	1.4	18

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37	Surface Resistance to Permeation through the Silicalite Single Crystal Membrane:Â Variation with Permeant. Journal of Physical Chemistry B, 2004, 108, 7801-7808.	1.2	35
38	The Diffusion Process of Methane through a Silicalite Single Crystal Membrane. Journal of Physical Chemistry B, 2002, 106, 5163-5168.	1.2	44