George K Papadopoulos

List of Publications by Year
in descending order

40 papers	1,328 citations	430874 18 h-index	345221 36 g-index
41 all docs	41 docs citations	41 times ranked	1316 citing authors

#	Article	IF	Citations
1	Prediction of Permeation Properties of CO2 and N2 through Silicalite via Molecular Simulations. Journal of Physical Chemistry B, 2001, 105, 777-788.	2.6	182
2	Water adsorption behaviour of CAU-10-H: a thorough investigation of its structureâ€“property relationships. Journal of Materials Chemistry A, 2016, 4, 11859-11869.	10.3	166
3	Determination of Micropore Size Distribution from Grand Canonical Monte Carlo Simulations and Experimental CO2 Isotherm Data. Langmuir, 1997, 13, 2795-2802.	3.5	108
4	Transport Diffusivity of N2and CO2in Silicalite:Â Coherent Quasielastic Neutron Scattering Measurements and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2004, 108, 12748-12756.	2.6	104
5	On the Impact of Sorbent Mobility on the Sorbed Phase Equilibria and Dynamics: A Study of Methane and Carbon Dioxide within the Zeolite Imidazolate Framework-8. Journal of Physical Chemistry C, 2012, 116, 201-207.	3.1	88
6	Diffusion in Fluid Catalytic Cracking Catalysts on Various Displacement Scales and Its Role in Catalytic Performance. Chemistry of Materials, 2005, 17, 2466-2474.	6.7	74
7	Atomistic Simulation Studies on the Dynamics and Thermodynamics of Nonpolar Molecules within the Zeolite Imidazolate Framework-8. Journal of Physical Chemistry B, 2010, 114, 2493-2503.	2.6	57
8	The Structure of Adsorbed CO2 in Slitlike Micropores at Low and High Temperature and the Resulting Micropore Size Distribution Based on GCMC Simulations. Journal of Colloid and Interface Science, 2000, 224, 272-290.	9.4	43
9	Sorption Thermodynamics of CO2, CH4, and Their Mixtures in the ITQ-1 Zeolite as Revealed by Molecular Simulations. Journal of Physical Chemistry B, 2006, 110, 22742-22753.	2.6	39
10	Probing the hydrogen equilibrium and kinetics in zeolite imidazolate frameworks via molecular dynamics and quasi-elastic neutron scattering experiments. Journal of Chemical Physics, 2013, 138, 034706.	3.0	38
11	Mesoscopic simulations of the diffusivity of ethane in beds of NaX zeolite crystals: Comparison with pulsed field gradient NMR measurements. Journal of Chemical Physics, 2007, 126, 094702.	3.0	28
12	Micropore size distributions from CO2 using grand canonical Monte Carlo at ambient temperatures: cylindrical versus slit pore geometries. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2004, 241, 127-135.	4.7	25
13	Molecular Dynamics Phenomena of Water in the Metalorganic Framework MIL-100(Al), as Revealed by Pulsed Field Gradient NMR and Atomistic Simulation. Journal of Physical Chemistry C, 2017, 121, 18065-18074.	3.1	25
14	Parallel tempering method for reconstructing isotropic and anisotropic porous media. Journal of Chemical Physics, 2002, 117, 5876-5884.	3.0	24
15	Characterization of nanoporous carbons by combining CO2 and H2 sorption data with the Monte Carlo simulations. Applied Surface Science, 2007, 253, 5715-5720.	6.1	23
16	Combined Atomistic Simulation and Quasielastic Neutron Scattering Study of the Low-Temperature Dynamics of Hydrogen and Deuterium Confined in NaX Zeolite. Journal of Physical Chemistry B, 2008, 112, 11708-11715.	2.6	23
17	Influence of orientational ordering transition on diffusion of carbon dioxide in carbon nanopores. Journal of Chemical Physics, 2001, 114, 8139-8144.	3.0	22
18	On the computation of long-range interactions in fluids under confinement: Application to pore systems with various types of spatial periodicity. Journal of Chemical Physics, 2007, 127, 164723.	3.0	22

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19	Atomistic Modeling of Water Thermodynamics and Kinetics within MIL-100(Fe). Journal of Physical Chemistry C, 2015, 119, 20074-20084.	3.1	21
20	Dimensionality reduction of free energy profiles of benzene in silicalite-1: calculation of diffusion coefficients using transition state theory. Molecular Simulation, 2014, 40, 80-100.	2.0	19
21	Simulation studies of methane, carbon dioxide, hydrogen and deuterium in ITQ-1 and NaX zeolites. Molecular Simulation, 2009, 35, 79-89.	2.0	18
22	Molecular Dynamics of Carbon Dioxide, Methane and Their Mixtures in a Zeolite Possessing Two Independent Pore Networks as Revealed by Computer Simulations. Journal of Physical Chemistry B, 2009, 113, 13761-13767.	2.6	18
23	Simulation Study of Sorption of CO₂and N₂with Application to the Characterization of Carbon Adsorbents. Molecular Simulation, 2001, 27, 441-456.	2.0	17
24	Intrinsic D₂/H₂ Selectivity of NaX Zeolite: Interplay between Adsorption and Kinetic Factors. Journal of Physical Chemistry C, 2015, 119, 15373-15380.	3.1	16
25	Unified formulation of isothermal adsorbate flow in mesoporous media over the full vapor pressure range. Journal of Membrane Science, 1995, 101, 127-133.	8.2	15
26	Pulsed-field gradient nuclear magnetic resonance study of transport properties of fluid catalytic cracking catalysts. Magnetic Resonance Imaging, 2005, 23, 233-237.	1.8	14
27	Molecular Dynamics Studies of Diffusion in Model Cylindrical Pores at Very Low Densities. Molecular Simulation, 1999, 22, 237-256.	2.0	12
28	Diffusivity of CH4In Model Silica Nanopores: Molecular Dynamics and Quasichemical Mean Field Theory. Molecular Simulation, 2005, 31, 57-66.	2.0	11
29	Constant Pressure Path Integral Gibbs Ensemble Monte Carlo Method. Journal of Chemical Theory and Computation, 2013, 9, 2922-2929.	5.3	11
30	Wasseradsorption und â€diffusion in SAPOâ€34 fÃ¼r die adsorptive WÃrmetransformation. Chemie-Ingenieur-Technik, 2016, 88, 372-378.	0.8	10
31	Experimental verification of a proposed unified formulation of adsorbate transport in mesoporous media over the full vapour pressure range. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 3217.	1.7	9
32	A Monte Carlo study on the structure of carbon dioxide adsorbed in microporous carbons.. Studies in Surface Science and Catalysis, 2002, 144, 545-552.	1.5	8
33	Model Study of the Effect of Pore Structure and Condensation on Multilayer Adsorbate Transport in Porous Media. Langmuir, 2007, 23, 12932-12936.	3.5	6
34	A second-order Markov process for modeling diffusive motion through spatial discretization. Journal of Chemical Physics, 2008, 128, 024504.	3.0	6
35	Diffusion via space discretization method to study the concentration dependence of self-diffusivity under confinement. Journal of Chemical Physics, 2010, 132, 134108.	3.0	6
36	Modeling the Hydration-Induced Structural Transitions of the SAPO-34 Zeolite and Their Impact on the Waterâ€™s Sorbed Phase Equilibrium and Dynamics. Journal of Physical Chemistry C, 2020, 124, 11480-11489.	3.1	4

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37	Binding Dynamics of siRNA with Selected Lipopeptides: A Computer-Aided Study of the Effect of Lipopeptidesâ€™ Functional Groups and Stereoisomerism. Journal of Chemical Theory and Computation, 2020, 16, 3842-3855.	5.3	4
38	Identification of hydrated phases in ALPO4-5, and explanation of their effect on the water sorption and dynamics. Microporous and Mesoporous Materials, 2021, , 111501.	4.4	4
39	Atomistic simulation of sorption in model pores with reduced spatial periodicity. Applied Surface Science, 2007, 253, 5606-5609.	6.1	3
40	A Localized Enantioselective Catalytic Site on Short DNA Sequences and Their Amphiphiles. Jacs Au, 2022, 2, 483-491.	7.9	3