## Grand Canonical Monte Carlo Simulation Study of Wate

Journal of Physical Chemistry B 112, 6390-6397 DOI: 10.1021/jp7097153

Citation Report

#	Article	IF	CITATIONS
1	A new scheme for perturbation contribution in density functional theory and application to solvation force and critical fluctuations. Journal of Chemical Physics, 2009, 131, 134702.	1.2	11
2	Molecular Simulation of Water Confined in Nanoporous Ca-silica. Materials Research Society Symposia Proceedings, 2009, 1227, 80501.	0.1	0
3	Molecular Simulations of Water and Paracresol in MFI Zeolite - A Monte Carlo Study. Langmuir, 2009, 25, 11598-11607.	1.6	12
4	Advanced Monte Carlo Approach To Study Evolution of Quartz Surface during the Dissolution Process. Journal of the American Chemical Society, 2009, 131, 9538-9546.	6.6	30
5	A realistic molecular model of cement hydrates. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 16102-16107.	3.3	734
6	Molecular simulations of adsorption and diffusion of RDX in IRMOF-1. Molecular Simulation, 2009, 35, 910-919.	0.9	28
7	Adsorption and Diffusion of Water, Methanol, and Ethanol in All-Silica DD3R: Experiments and Simulation. Journal of Physical Chemistry C, 2009, 113, 14290-14301.	1.5	69
8	Evaluation of various water models for simulation of adsorption in hydrophobic zeolites. Molecular Simulation, 2009, 35, 1067-1076.	0.9	60
9	Evaluation of confinement effects in zeolites under Henry's adsorption regime. Applied Surface Science, 2010, 256, 5305-5310.	3.1	12
10	Adsorption and Phase Behaviour in Nanochannels and Nanotubes. , 2010, , .		23
12	Water behaviour in nanoporous aluminosilicates. Journal of Physics Condensed Matter, 2010, 22, 284115.	0.7	6
13	Molecular simulation of water confined in nanoporous silica. Journal of Physics Condensed Matter, 2010, 22, 284110.	0.7	111
14	Molecular Computations of Adsorption in Nanoporous Materials. , 2010, , 69-100.		2
15	Hydrogen Bonding Effects in Adsorption of Waterâ^'Alcohol Mixtures in Zeolites and the Consequences for the Characteristics of the Maxwellâ^'Stefan Diffusivities. Langmuir, 2010, 26, 10854-10867.	1.6	127
16	Toward an Accurate Modeling of the Waterâ^'Zeolite Interaction: Calibrating the DFT Approach. Journal of Physical Chemistry Letters, 2010, 1, 763-768.	2.1	12
17	Role of Intrasurface Hydrogen Bonding on Silica Dissolution. Journal of Physical Chemistry C, 2010, 114, 2267-2272.	1.5	13
18	Glassy Nature of Water in an Ultraconfining Disordered Material: The Case of Calciumâ^'Silicateâ^'Hydrate. Journal of the American Chemical Society, 2011, 133, 2499-2510.	6.6	232
19	Monte Carlo Simulation of Water Adsorption in Hydrophobic MFI Zeolites with Hydrophilic Sites.	1.6	53

#	ARTICLE	IF	CITATIONS
20	A Computational Investigation into the Suitability of Purely Siliceous Zeolites as Reverse Osmosis Membranes. Journal of Physical Chemistry C, 2011, 115, 4063-4075.	1.5	37
21	Simulations of the Quartz(101ì1)/Water Interface: A Comparison of Classical Force Fields, Ab Initio Molecular Dynamics, and X-ray Reflectivity Experiments. Journal of Physical Chemistry C, 2011, 115, 2076-2088.	1.5	183
22	Molecular Simulation of a Zn–Triazamacrocyle Metal–Organic Frameworks Family with Extraframework Anions. Journal of Physical Chemistry C, 2012, 116, 2952-2959.	1.5	5
23	Confined Water Dissociation in Microporous Defective Silicates: Mechanism, Dipole Distribution, and Impact on Substrate Properties. Journal of the American Chemical Society, 2012, 134, 2208-2215.	6.6	264
24	Solvated calcium ions in charged silica nanopores. Journal of Chemical Physics, 2012, 137, 064706.	1.2	32
25	Thermodynamics of Water Confined in Porous Calcium-Silicate-Hydrates. Langmuir, 2012, 28, 11422-11432.	1.6	157
26	Adsorption of CO <sub>2</sub> , CH <sub>4</sub> , and H <sub>2</sub> O in Zeolite ZSM-5 Studied Using In Situ ATR-FTIR Spectroscopy. Journal of Physical Chemistry C, 2013, 117, 16972-16982.	1.5	92
27	Investigating the influence of diffusional coupling on mixture permeation across porous membranes. Journal of Membrane Science, 2013, 430, 113-128.	4.1	44
29	Simulating Adsorptive Expansion of Zeolites: Application to Biomass-Derived Solutions in Contact with Silicalite. Langmuir, 2013, 29, 4866-4876.	1.6	14
30	The effects of partial charges and water models on water adsorption in nanostructured zeolites, application of PN-TrAz potential in parallel GCMC. Molecular Simulation, 2013, 39, 495-504.	0.9	12
31	Upgrading of Simulated Syngas by Using a Nanoporous Silica Membrane Reactor. Chemical Engineering and Technology, 2013, 36, 650-656.	0.9	9
32	Acid Gases in CO2-rich Subsurface Geologic Environments. Reviews in Mineralogy and Geochemistry, 2013, 77, 361-398.	2.2	14
33	Isotherms of Fluids in Native and Defective Zeolite and Alumino-Phosphate Crystals: Monte-Carlo Simulations with "On-the-Flyâ€ <i>ab initio</i> Electrostatic Potential. Oil and Gas Science and Technology, 2013, 68, 299-307.	1.4	2
34	10. Acid Gases in CO <sub>2</sub> -rich Subsurface Geologic Environments. , 2013, , 361-398.		2
35	Anomalous composition-dependent dynamics of nanoconfined water in the interlayer of disordered calcium-silicates. Journal of Chemical Physics, 2014, 140, 054515.	1.2	121
36	A simple grand canonical approach to compute the vapor pressure of bulk and finite size systems. Journal of Chemical Physics, 2014, 140, 064111.	1.2	25
37	Coarse-Graining of Adsorption in Microporous Materials: Relation between Occupancy Distributions and Local Partition Functions. Journal of Physical Chemistry C, 2014, 118, 28711-28719.	1.5	3
38	Adsorption by Clays, Pillared Clays, Zeolites and Aluminophosphates. , 2014, , 467-527.		15

CITATION REPORT

CITATION REPORT

#	Article	IF	CITATIONS
39	Porous Inorganic Membranes for CO <sub>2</sub> Capture: Present and Prospects. Chemical Reviews, 2014, 114, 1413-1492.	23.0	481
40	Molecular simulation of "hydrolytic weakeningâ€! A case study on silica. Acta Materialia, 2014, 80, 264-277.	3.8	50
41	Water Stability and Adsorption in Metal–Organic Frameworks. Chemical Reviews, 2014, 114, 10575-10612.	23.0	1,951
42	Fluid adsorption in linear pores: a molecular simulation study of the influence of heterogeneities on the hysteresis loop and the distribution of metastable states. Molecular Simulation, 2014, 40, 690-697.	0.9	6
43	Nanoconfined gases, liquids and liquid crystals in porous materials. Molecular Simulation, 2014, 40, 698-712.	0.9	5
44	Molecular dynamics study of water and ions transport in nano-pore of layered structure: A case study of tobermorite. Microporous and Mesoporous Materials, 2014, 195, 9-20.	2.2	141
45	Structural, dynamic and mechanical evolution of water confined in the nanopores of disordered calcium silicate sheets. Microfluidics and Nanofluidics, 2015, 19, 1309-1323.	1.0	31
46	Reactive Molecular Simulation on Water Confined in the Nanopores of the Calcium Silicate Hydrate Gel: Structure, Reactivity, and Mechanical Properties. Journal of Physical Chemistry C, 2015, 119, 1346-1358.	1.5	194
47	Water transport in the nano-pore of the calcium silicate phase: reactivity, structure and dynamics. Physical Chemistry Chemical Physics, 2015, 17, 1411-1423.	1.3	75
48	Reactive force field simulation on polymerization and hydrolytic reactions in calcium aluminate silicate hydrate (C–A–S–H) gel: structure, dynamics and mechanical properties. RSC Advances, 2015, 5, 448-461.	1.7	78
49	Uniaxial tension study of calcium silicate hydrate (C–S–H): structure, dynamics and mechanical properties. Materials and Structures/Materiaux Et Constructions, 2015, 48, 3811-3824.	1.3	84
50	Transferable force-field for modelling of CO <sub>2</sub> , N <sub>2</sub> , O <sub>2</sub> and Ar in all silica and Na <sup>+</sup> exchanged zeolites. Modelling and Simulation in Materials Science and Engineering, 2016, 24, 045002.	0.8	53
51	Transient effects of drying creep in nanoporous solids: understanding the effects of nanoscale energy barriers. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2016, 472, 20160490.	1.0	11
52	Reactive molecular simulation on the ordered crystal and disordered glass of the calcium silicate hydrate gel. Ceramics International, 2016, 42, 4333-4346.	2.3	34
53	Coarse-grained molecular dynamics simulations of capillary evaporation of water confined in hydrophilic mesopores. Molecular Physics, 2016, 114, 884-894.	0.8	7
54	Molecular Simulation of the Ions Ultraconfined in the Nanometer-Channel of Calcium Silicate Hydrate: Hydration Mechanism, Dynamic Properties, and Influence on the Cohesive Strength. Inorganic Chemistry, 2017, 56, 1881-1896.	1.9	25
55	Stability and Vapor Pressure of Aqueous Aggregates and Aerosols Containing a Monovalent Ion. Journal of Physical Chemistry A, 2017, 121, 2597-2602.	1.1	3
56	A molecular dynamics study of the interaction of water with the external surface of silicalite-1. Physical Chemistry Chemical Physics, 2017, 19, 2950-2960.	1.3	28

ARTICLE IF CITATIONS # Multiscale simulation approach to heat and mass transfer properties of nanostructured materials 57 1.8 12 for sorption heat storage. Energy Procedia, 2017, 126, 509-516. Numerical evidence of heterogeneity and nanophases in a binary liquid confined at the nanoscale. Molecular Simulation, 2018, 44, 728-735. A novel temperature swing adsorption process for natural gas purification: Part I, model 59 3.9 14 development. Separation and Purification Technology, 2018, 203, 124-142. A nanoscale perspective on the effects of transverse microprestress on drying creep of nanoporous solids. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2018, 474, 20170570. Isosteric heat of adsorption at zero coverage for AQSOA-Z01/Z02/Z05 zeolites and water systems. 61 2.2 23 Microporous and Mesoporous Materials, 2018, 260, 201-207. Nano-scale mechanical properties investigation of C-S-H from hydrated tri-calcium silicate by nano-indentation and molecular dynamics simulation. Construction and Building Materials, 2018, 189, 3.2 44 Influence of surface commensurability on the structure and relaxation dynamics of a confined 63 1.2 10 monatomic fluid. Journal of Chemical Physics, 2018, 149, 064503. Defectâ€Mediated Ordering of Condensed Water Structures in Microporous Zeolites. Angewandte 64 1.6 Chemie, 2019, 131, 16574-16578. Defectâ€Mediated Ordering of Condensed Water Structures in Microporous Zeolites. Angewandte 7.2 38 65 Chemie - International Edition, 2019, 58, 16422-16426. Mechanistic correlation between water infiltration and framework hydrophilicity in MFI zeolites. 1.6 Scientific Reports, 2019, 9, 18429. A priori predictions of type I and type V isotherms by the rigid adsorbent lattice fluid. Adsorption, 67 1.4 13 2020, 26, 989-1000. Dynamics of confined water and its interplay with alkali cations in sodium aluminosilicate hydrate gel: insights from reactive force field molecular dynamics. Physical Chemistry Chemical Physics, 2020, 22, 23707-23724. 1.3 68 Fracture toughness of fly ash-based geopolymer gels: Evaluations using nanoindentation experiment 69 3.2 22 and molecular dynamics simulation. Construction and Building Materials, 2020, 262, 120797. Numerical Simulation of Adsorption of Organic Inhibitors on C-S-H Gel. Crystals, 2020, 10, 742. 1.0 Elucidating the constitutive relationship of calciumâ€"silicateâ€"hydrate gel using high throughput 71 12 1.6 reactive molecular simulations and machine learning. Scientific Reports, 2020, 10, 21336. Efficient Downstream Processing of Renewable Alcohols Using Zeolite Adsorbents. Structure and Bonding, 2020, , 85-119. Fracture toughness of sodium aluminosilicate hydrate (NASH) gels: Insights from molecular dynamics 73 1.1 10 simulations. Journal of Applied Physics, 2020, 127, . Utilization of zeolite as a potential multi-functional proppant for CO2 enhanced shale gas recovery 74 and CO2 sequestration: A molecular simulation study of the impact of water on adsorption in zeolite and organic matter. Fuel, 2021, 292, 120312.

CITATION REPORT

#	Article	IF	CITATIONS
75	Capturing renewable isobutanol from model vapor mixtures using an all-silica beta zeolite. Chemical Engineering Journal, 2021, 412, 128658.	6.6	9
76	Tailoring Zirconium-based metal organic frameworks for enhancing Hydrophilic/Hydrophobic Characteristics: Simulation and experimental investigation. Journal of Molecular Liquids, 2021, 341, 117381.	2.3	7
77	Modeling the Calcium Silicate Hydrate by Molecular Simulation. , 2020, , 55-86.		0
78	Improving the adhesion properties of cement/epoxy interface using graphene-based nanomaterials: Insights from molecular dynamics simulation. Cement and Concrete Composites, 2022, 134, 104801.	4.6	19
79	Molecular Dynamics Simulations of Chloride and Sulfate Ion Transport in C-S-H gel and Î <sup>3</sup> -FeOOH Nanopores. Journal of Advanced Concrete Technology, 2022, 20, 720-731.	0.8	1