Alain H Fuchs

List of Publications by Year
in descending order

120 papers	7,268 citations	50170 46 h-index	56606 83 g-index
129 all docs	129 docs citations	129 times ranked	5457 citing authors

#	Article	IF	Citations
1	Open questions on water confined in nanoporous materials. Communications Chemistry, 2021, 4, .	2.0	15
2	Structure, Dynamics, and Thermodynamics of Intruded Electrolytes in ZIF-8. Journal of Physical Chemistry C, 2019, 123, 15589-15598.	1.5	22
3	On the use of the IAST method for gas separation studies in porous materials with gate-opening behavior. Adsorption, 2018, 24, 233-241.	1.4	30
4	Impacts of the Imidazolate Linker Substitution (CH₃, Cl, or Br) on the Structural and Adsorptive Properties of ZIF-8. Journal of Physical Chemistry C, 2018, 122, 26945-26955.	1.5	40
5	Interplay between defects, disorder and flexibility in metal-organic frameworks. Nature Chemistry, 2017, 9, 11-16.	6.6	342
6	Forced intrusion of water and aqueous solutions in microporous materials: from fundamental thermodynamics to energy storage devices. Chemical Society Reviews, 2017, 46, 7421-7437.	18.7	78
7	Mechanism of water adsorption in the large pore form of the gallium-based MIL-53 metal-organic framework. Microporous and Mesoporous Materials, 2016, 222, 145-152.	2.2	14
8	Flexibility and disorder in metalâ€“organic frameworks. Dalton Transactions, 2016, 45, 4058-4059.	1.6	26
9	Adsorption deformation of microporous composites. Dalton Transactions, 2016, 45, 4136-4140.	1.6	14
10	Computational characterization and prediction of metalâ€“organic framework properties. Coordination Chemistry Reviews, 2016, 307, 211-236.	9.5	206
11	Hydrothermal Breakdown of Flexible Metalâ€“Organic Frameworks: A Study by First-Principles Molecular Dynamics. Journal of Physical Chemistry Letters, 2015, 6, 4365-4370.	2.1	23
12	Softening upon Adsorption in Microporous Materials: A Counterintuitive Mechanical Response. Journal of Physical Chemistry Letters, 2015, 6, 4265-4269.	2.1	20
13	A thermodynamic description of the adsorption-induced structural transitions in flexible MIL-53 metal-organic framework. Molecular Physics, 2014, 112, 1257-1261.	0.8	18
14	Comment on â€œVolume shrinkage of a metalâ€“organic framework host induced by the dispersive attraction of guest gas moleculesâ€• Physical Chemistry Chemical Physics, 2014, 16, 4394.	1.3	8
15	Water Adsorption in Flexible Gallium-Based MIL-53 Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2014, 118, 5397-5405.	1.5	55
16	What makes zeolitic imidazolate frameworks hydrophobic or hydrophilic? The impact of geometry and functionalization on water adsorption. Physical Chemistry Chemical Physics, 2014, 16, 9940-9949.	1.3	142
17	Metalâ€“organic frameworks with wine-rack motif: What determines their flexibility and elastic properties?. Journal of Chemical Physics, 2013, 138, 174703.	1.2	139
18	Adsorption induced transitions in soft porous crystals: An osmotic potential approach to multistability and intermediate structures. Journal of Chemical Physics, 2013, 138, 174706.	1.2	74

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19	Hydrothermal and Mechanical Stability of Metal-Organic Frameworks. , 2013, , .		0
20	Adsorption Deformation and Structural Transitions in Metalâ€“Organic Frameworks: From the Unit Cell to the Crystal. Journal of Physical Chemistry Letters, 2013, 4, 3198-3205.	2.1	148
21	Temperature-Induced Structural Transitions in the Gallium-Based MIL-53 Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2013, 117, 8180-8188.	1.5	59
22	Investigating the Pressure-Induced Amorphization of Zeolitic Imidazolate Framework ZIF-8: Mechanical Instability Due to Shear Mode Softening. Journal of Physical Chemistry Letters, 2013, 4, 1861-1865.	2.1	148
23	Adsorption-Induced Breathing Transitions in Metal-Organic Frameworks. , 2013, , .		0
24	Understanding adsorption-induced structural transitions in metal-organic frameworks: From the unit cell to the crystal. Journal of Chemical Physics, 2012, 137, 184702.	1.2	35
25	Anisotropic Elastic Properties of Flexible Metal-Organic Frameworks: How Soft are Soft Porous Crystals?. Physical Review Letters, 2012, 109, 195502.	2.9	265
26	Molecular Simulation of a Znâ€“Triazamacrocyle Metalâ€“Organic Frameworks Family with Extraframework Anions. Journal of Physical Chemistry C, 2012, 116, 2952-2959.	1.5	5
27	Chemistry in France: A Hotbed for New Schools of Thought. Angewandte Chemie - International Edition, 2012, 51, 12632-12633.	7.2	0
28	Predicting Mixture Coadsorption in Soft Porous Crystals: Experimental and Theoretical Study of CO₂/CH₄ in MIL-53(Al). Langmuir, 2012, 28, 494-498.	1.6	45
29	Experiment and Theory of Low-Pressure Nitrogen Adsorption in Organic Layers Supported or Grafted on Inorganic Adsorbents: Toward a Tool To Characterize Surfaces of Hybrid Organic/Inorganic Systems. Langmuir, 2012, 28, 9526-9534.	1.6	15
30	How Can a Hydrophobic MOF be Waterâ€Unstable? Insight into the Hydration Mechanism of IRMOFs. ChemPhysChem, 2012, 13, 3497-3503.	1.0	116
31	Structural Changes in Nanoporous MFI Zeolites Induced by Tetrachloroethene Adsorption: A Joint Experimental and Simulation Study. Journal of Physical Chemistry C, 2011, 115, 3854-3865.	1.5	9
32	Structural Transitions in MIL-53 (Cr): View from Outside and Inside. Langmuir, 2011, 27, 4734-4741.	1.6	143
33	Mechanism of Breathing Transitions in Metalâ€“Organic Frameworks. Journal of Physical Chemistry Letters, 2011, 2, 2033-2037.	2.1	74
34	Understanding the Equilibrium Ion Exchange Properties in Faujasite Zeolite from Monte Carlo Simulations. Journal of Physical Chemistry B, 2011, 115, 15059-15066.	1.2	37
35	Thermodynamic Methods and Models to Study Flexible Metalâ€“Organic Frameworks. ChemPhysChem, 2011, 12, 247-258.	1.0	105
36	Thermodynamic analysis of the breathing of amino-functionalized MIL-53(Al) upon CO2 adsorption. Microporous and Mesoporous Materials, 2011, 140, 108-113.	2.2	78

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37	Evidence of a framework induced cation redistribution upon water adsorption in cobalt exchanged X faujasite zeolite: A joint experimental and simulation study. Microporous and Mesoporous Materials, 2011, 138, 45-50.	2.2	46
38	Stress-Based Model for the Breathing of Metalâ^'Organic Frameworks. Journal of Physical Chemistry Letters, 2010, 1, 445-449.	2.1	209
39	The Behavior of Flexible MIL-53(Al) upon CH₄and CO₂Adsorption. Journal of Physical Chemistry C, 2010, 114, 22237-22244.	1.5	197
40	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
41	Understanding the Effect of Confinement on the Liquidâ^'Gas Transition: A Study of Adsorption Isotherms in a Family of Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2010, 114, 21631-21637.	1.5	27
42	Water adsorption in hydrophobic MOF channels. Physical Chemistry Chemical Physics, 2010, 12, 8123.	1.3	72
43	Thermodynamic study of water confinement in hydrophobic zeolites by Monte Carlo simulations. Molecular Simulation, 2009, 35, 24-30.	0.9	27
44	Breathing Transitions in MILâ€53(Al) Metalâ€"Organic Framework Upon Xenon Adsorption. Angewandte Chemie - International Edition, 2009, 48, 8314-8317.	7.2	176
45	Unusual Hysteresis Loop in the Adsorptionâ^'Desorption of Water in NaY Zeolite at Very Low Pressure. Journal of Physical Chemistry C, 2009, 113, 8287-8295.	1.5	34
46	Double Structural Transition in Hybrid Material MIL-53 upon Hydrocarbon Adsorption: The Thermodynamics Behind the Scenes. Journal of the American Chemical Society, 2009, 131, 3442-3443.	6.6	72
47	Prediction of Breathing and Gate-Opening Transitions Upon Binary Mixture Adsorption in Metalâ^'Organic Frameworks. Journal of the American Chemical Society, 2009, 131, 11329-11331.	6.6	144
48	Water nanodroplets confined in zeolite pores. Faraday Discussions, 2009, 141, 377-398.	1.6	71
49	A molecular simulation study of the distribution of cation inÂzeolites. Adsorption, 2008, 14, 743-754.	1.4	32
50	Does Water Condense in Hydrophobic Cavities? A Molecular Simulation Study of Hydration in Heterogeneous Nanopores. Journal of Physical Chemistry C, 2008, 112, 10435-10445.	1.5	63
51	Thermodynamics of Guest-Induced Structural Transitions in Hybrid Organicâ^'Inorganic Frameworks. Journal of the American Chemical Society, 2008, 130, 14294-14302.	6.6	299
52	Thermodynamics of water intrusion in nanoporous hydrophobic solids. Physical Chemistry Chemical Physics, 2008, 10, 4817.	1.3	103
53	Structural changes in nanoporous solids due to fluid adsorption: thermodynamic analysis and Monte Carlo simulations. Chemical Communications, 2008, , 3275.	2.2	38
54	Thermodynamic study of water intrusion in hydrophobic zeolites by Monte Carlo simulations. Studies in Surface Science and Catalysis, 2008, 174, 683-688.	1.5	3

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55	Influence of defects on the water intrusion in silicalite-1 zeolite: confrontation of experimental and molecular simulation results. Studies in Surface Science and Catalysis, 2008, 174, 561-564.	1.5	6
56	The Effect of Local Defects on Water Adsorption in Silicalite-1 Zeolite:â€‰ A Joint Experimental and Molecular Simulation Study. Langmuir, 2007, 23, 10131-10139.	1.6	181
57	Molecular simulation applied to fluid properties in the oil and gas industry. Molecular Simulation, 2007, 33, 287-304.	0.9	34
58	Adsorption of n-alkanes in faujasite zeolites: molecular simulation study and experimental measurements. Adsorption, 2007, 13, 439-451.	1.4	38
59	Molecular simulation studies of water physisorption in zeolites. Physical Chemistry Chemical Physics, 2006, 8, 5396.	1.3	139
60	Adsorption of n-Alkanes in Faujasite Zeolites: Molecular Simulation Study and Experimental Measurements. Adsorption Science and Technology, 2006, 24, 713-735.	1.5	6
61	Adsorption of water in zeolite sodium-faujasite. Comptes Rendus Chimie, 2005, 8, 485-490.	0.2	49
62	Water Condensation in Hydrophobic Nanopores. Angewandte Chemie - International Edition, 2005, 44, 5310-5313.	7.2	155
63	Adsorption of Water and Aromatics in Faujasite Zeolites: A Molecular Simulation Study. Adsorption, 2005, 11, 279-282.	1.4	14
64	Adsorption of Various Hydrocarbons in Siliceous Zeolites: A Molecular Simulation Study. Adsorption, 2005, 11, 379-382.	1.4	11
65	Unexpected Si:Al Effect on the Binary Mixtures Liquid Phase Adsorption Selectivities in Faujasite Zeolites. Journal of the American Chemical Society, 2005, 127, 11600-11601.	6.6	21
66	Torsion-induced phase transitions in fluids confined between chemically decorated substrates. Journal of Chemical Physics, 2004, 121, 9077-9086.	1.2	5
67	Adsorption of Linear Alkanes in Zeolite Ferrierite from Molecular Simulations. Molecular Simulation, 2004, 30, 593-599.	0.9	8
68	Monte Carlo versus molecular dynamics simulations in heterogeneous systems: An application to the n-pentane liquid-vapor interface. Journal of Chemical Physics, 2004, 121, 12559.	1.2	71
69	A Numerical Evidence for Nonframework Cation Redistribution Upon Water Adsorption in Faujasite Zeolite. ChemPhysChem, 2004, 5, 1791-1793.	1.0	37
70	Distribution of Sodium Cations in Faujasite-Type Zeolite:Â A Canonical Parallel Tempering Simulation Study. Journal of Physical Chemistry B, 2004, 108, 399-404.	1.2	79
71	Fluid phase transitions at chemically heterogeneous, nonplanar solid substrates: Surface versus confinement effects. Journal of Chemical Physics, 2003, 118, 1453-1465.	1.2	25
72	Nanoscopic liquid bridges exposed to a torsional strain. Physical Review E, 2003, 68, 066103.	0.8	5

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73	New optimization method for intermolecular potentials: Optimization of a new anisotropic united atoms potential for olefins: Prediction of equilibrium properties. Journal of Chemical Physics, 2003, 118, 3020-3034.	1.2	142
74	Structure of ultra-thin confined alkane films from Monte Carlo simulations. Molecular Physics, 2002, 100, 2109-2119.	0.8	14
75	Monte Carlo simulation of a complex fluid confined to a pore with nanoscopically rough walls. Journal of Chemical Physics, 2002, 116, 5816-5824.	1.2	36
76	Monte Carlo simulation of branched alkanes and long chain n -alkanes with anisotropic united atoms intermolecular potential. Molecular Simulation, 2002, 28, 317-336.	0.9	79
77	Cation distribution in faujasite-type zeolites: A test of semi-empirical force fields for Na cations. Molecular Simulation, 2002, 28, 1049-1062.	0.9	18
78	Fluids confined by nanopatterned substrates of low symmetry. Molecular Physics, 2002, 100, 2971-2982.	0.8	11
79	Direct Monte Carlo simulations of the equilibrium properties ofn-pentane liquidâ€“vapor interface. Journal of Chemical Physics, 2002, 116, 8106-8117.	1.2	75
80	Vapour-Liquid Phase Equilibria of n-alkanes by Direct Monte Carlo Simulations. Molecular Simulation, 2001, 27, 99-114.	0.9	41
81	Molecular Simulation of Adsorption of Guest Molecules in Zeolitic Materials: A Comparative Study of Intermolecular Potentials. Molecular Simulation, 2001, 27, 371-385.	0.9	8
82	Adsorption of Guest Molecules in Zeolitic Materials: Computational Aspects. Journal of Physical Chemistry B, 2001, 105, 7375-7383.	1.2	217
83	Placement of cations in NaX faujasite-type zeolite using (N,V,T) Monte Carlo simulations. Chemical Communications, 2001, , 2200-2201.	2.2	25
84	Structure and solvation forces in confined alkane films. Physical Chemistry Chemical Physics, 2001, 3, 1155-1159.	1.3	37
85	Direct calculation of bubble points for alkane mixtures by molecular simulation. Molecular Physics, 2001, 99, 1423-1434.	0.8	20
86	Molecular simulation of adsorption equilibria of xylene isomer mixtures in faujasite zeolites. A study of the cation exchange effect on adsorption selectivity. Physical Chemistry Chemical Physics, 2001, 3, 80-86.	1.3	35
87	A Simple Model for Predicting the Na+Distribution in Anhydrous NaY and NaX Zeolites. Journal of Physical Chemistry B, 2001, 105, 9569-9575.	1.2	120
88	Prediction of thermodynamic derivative properties of fluids by Monte Carlo simulation. Physical Chemistry Chemical Physics, 2001, 3, 4333-4339.	1.3	110
89	Optimization of the anisotropic united atoms intermolecular potential forn-alkanes. Journal of Chemical Physics, 2000, 112, 5499-5510.	1.2	270
90	On the role of the definition of potential models in Gibbs ensemble phase equilibria simulations of the H₂S-pentane mixture. Molecular Physics, 2000, 98, 1895-1905.	0.8	25

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91	Molecular Simulation of Vapour-Liquid Coexistence Curves for Hydrogen Sulfide-Alkane and Carbon Dioxide-Alkane Mixtures. Molecular Simulation, 1999, 22, 351-368.	0.9	28
92	From molecular clusters to bulk matter. II. Crossover from icosahedral to crystalline structures in CO2 clusters. Journal of Chemical Physics, 1999, 111, 2095-2102.	1.2	32
93	Monte Carlo simulations of squalane in the Gibbs ensemble. Fluid Phase Equilibria, 1999, 155, 167-176.	1.4	16
94	Molecular Simulation of p-Xylene and m-Xylene Adsorption in Y Zeolites. Single Components and Binary Mixtures Study. Langmuir, 1999, 15, 8678-8685.	1.6	62
95	Monte Carlo simulations of nanoconfined n-decane films. Physical Chemistry Chemical Physics, 1999, 1, 4083.	1.3	25
96	Computational Study ofp-Xylene/m-Xylene Mixtures Adsorbed in NaY Zeolite. Journal of Physical Chemistry B, 1998, 102, 9224-9233.	1.2	75
97	Stick-slip phase transitions in confined solidlike films from an equilibrium perspective. Physical Review E, 1998, 57, 1621-1635.	0.8	34
98	From molecular clusters to bulk matter. I. Structure and thermodynamics of small CO2, N2, and SF6 clusters. Journal of Chemical Physics, 1998, 109, 329-337.	1.2	64
99	Rheology of model confined ultrathin fluid films. I. Statistical mechanics of the surface force apparatus experiments. Journal of Chemical Physics, 1997, 106, 7295-7302.	1.2	44
100	The Melting Phase Transition in Small Carbon Dioxide Clusters. Molecular Simulation, 1997, 19, 285-299.	0.9	6
101	Grand canonical Monte Carlo simulations of adsorption of mixtures of xylene molecules in faujasite zeolites. Faraday Discussions, 1997, 106, 307-323.	1.6	68
102	Vapour-Liquid Phase Equilibria Predictions of Methaneâ€“Alkane Mixtures by Monte Carlo Simulation. Molecular Simulation, 1997, 19, 1-15.	0.9	79
103	The Adsorption of Argon and Nitrogen in Silicalite-1 Zeolite: A Grand Canonical Monte-Carlo study. Molecular Simulation, 1996, 17, 255-288.	0.9	30
104	Grand Canonical Monte Carlo Simulations of Adsorption of Polar and Nonpolar Molecules in NaY Zeolite. Langmuir, 1996, 12, 4768-4783.	1.6	58
105	Numerical Evidence of an Embryonic Orientational Phase Transition in Small Nitrogen Clusters. Physical Review Letters, 1996, 76, 4336-4339.	2.9	28
106	Molecular Simulation Study of the Structural Rearrangement of Methane Adsorbed in Aluminophosphate AlPO4-5. The Journal of Physical Chemistry, 1996, 100, 9006-9013.	2.9	75
107	The temperature-size phase diagram of large SF6 clusters by computer simulation. Chemical Physics Letters, 1994, 218, 122-127.	1.2	26
108	The phase transitions of sulphur hexafluoride by molecular dynamics simulation. Molecular Physics, 1994, 81, 1165-1176.	0.8	4

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109			