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	Interplay between defects, disorder and flexibility in metal-organic frameworks. Nature Chemistry, 2017, 9, 11-16.	6.6	342
2	Thermodynamics of Guest-Induced Structural Transitions in Hybrid Organicâ"Inorganic Frameworks. Journal of the American Chemical Society, 2008, 130, 14294-14302.	6.6	299
3	Optimization of the anisotropic united atoms intermolecular potential forn-alkanes. Journal of Chemical Physics, 2000, 112, 5499-5510.	1.2	270
4	Anisotropic Elastic Properties of Flexible Metal-Organic Frameworks: How Soft are Soft Porous Crystals?. Physical Review Letters, 2012, 109, 195502.	2.9	265
5	Adsorption of Guest Molecules in Zeolitic Materials: Computational Aspects. Journal of Physical Chemistry B, 2001, 105, 7375-7383.	1.2	217
6	Stress-Based Model for the Breathing of Metalâ"Organic Frameworks. Journal of Physical Chemistry Letters, 2010, 1, 445-449.	2.1	209
7	Computational characterization and prediction of metalâ€"organic framework properties. Coordination Chemistry Reviews, 2016, 307, 211-236.	9.5	206
8	The Behavior of Flexible MIL-53(Al) upon CH₄and CO₂Adsorption. Journal of Physical Chemistry C, 2010, 114, 22237-22244.	1.5	197
9	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
10	Breathing Transitions in MILâ€53(Al) Metalâ€"Organic Framework Upon Xenon Adsorption. Angewandte Chemie - International Edition, 2009, 48, 8314-8317.	7.2	176
11	Water Condensation in Hydrophobic Nanopores. Angewandte Chemie - International Edition, 2005, 44, 5310-5313.	7.2	155
12	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
13	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
14	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
15	Structural Transitions in MIL-53 (Cr): View from Outside and Inside. Langmuir, 2011, 27, 4734-4741.	1.6	143
16	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
17	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
18	Molecular simulation studies of water physisorption in zeolites. Physical Chemistry Chemical Physics, 2006, 8, 5396.	1.3	139

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19	Metalâ€“organic frameworks with wine-rack motif: What determines their flexibility and elastic properties?. Journal of Chemical Physics, 2013, 138, 174703.	1.2	139
20	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
21	How Can a Hydrophobic MOF be Waterâ€Unstable? Insight into the Hydration Mechanism of IRMOFs. ChemPhysChem, 2012, 13, 3497-3503.	1.0	116
22	Prediction of thermodynamic derivative properties of fluids by Monte Carlo simulation. Physical Chemistry Chemical Physics, 2001, 3, 4333-4339.	1.3	110
23	Thermodynamic Methods and Models to Study Flexible Metalâ€“Organic Frameworks. ChemPhysChem, 2011, 12, 247-258.	1.0	105
24	Thermodynamics of water intrusion in nanoporous hydrophobic solids. Physical Chemistry Chemical Physics, 2008, 10, 4817.	1.3	103
25	Vapour-Liquid Phase Equilibria Predictions of Methaneâ€“Alkane Mixtures by Monte Carlo Simulation. Molecular Simulation, 1997, 19, 1-15.	0.9	79
26	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
27	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
28	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
29	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
30	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
31	Computational Study ofp-Xylene/m-Xylene Mixtures Adsorbed in NaY Zeolite. Journal of Physical Chemistry B, 1998, 102, 9224-9233.	1.2	75
32	Direct Monte Carlo simulations of the equilibrium properties ofn-pentane liquidâ€“vapor interface. Journal of Chemical Physics, 2002, 116, 8106-8117.	1.2	75
33	Mechanism of Breathing Transitions in Metalâ€“Organic Frameworks. Journal of Physical Chemistry Letters, 2011, 2, 2033-2037.	2.1	74
34	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
35	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
36	Water adsorption in hydrophobic MOF channels. Physical Chemistry Chemical Physics, 2010, 12, 8123.	1.3	72

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37	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
38	Water nanodroplets confined in zeolite pores. Faraday Discussions, 2009, 141, 377-398.	1.6	71
39	Grand canonical Monte Carlo simulations of adsorption of mixtures of xylene molecules in faujasite zeolites. Faraday Discussions, 1997, 106, 307-323.	1.6	68
40	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
41	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
42	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
43	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
44	Grand Canonical Monte Carlo Simulations of Adsorption of Polar and Nonpolar Molecules in NaY Zeolite. Langmuir, 1996, 12, 4768-4783.	1.6	58
45	Water Adsorption in Flexible Gallium-Based MIL-53 Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2014, 118, 5397-5405.	1.5	55
46	Adsorption of water in zeolite sodium-faujasite. Comptes Rendus Chimie, 2005, 8, 485-490.	0.2	49
47	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
48	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
49	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
50	Vapour-Liquid Phase Equilibria of n-alkanes by Direct Monte Carlo Simulations. Molecular Simulation, 2001, 27, 99-114.	0.9	41
51	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
52	Adsorption of n-alkanes in faujasite zeolites: molecular simulation study and experimental measurements. Adsorption, 2007, 13, 439-451.	1.4	38
53	Structural changes in nanoporous solids due to fluid adsorption: thermodynamic analysis and Monte Carlo simulations. Chemical Communications, 2008, , 3275.	2.2	38
54	Structure and solvation forces in confined alkane films. Physical Chemistry Chemical Physics, 2001, 3, 1155-1159.	1.3	37

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55	A Numerical Evidence for Nonframework Cation Redistribution Upon Water Adsorption in Faujasite Zeolite. ChemPhysChem, 2004, 5, 1791-1793.	1.0	37
56	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
57	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
58	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
59	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
60	Stick-slip phase transitions in confined solidlike films from an equilibrium perspective. Physical Review E, 1998, 57, 1621-1635.	0.8	34
61	Molecular simulation applied to fluid properties in the oil and gas industry. Molecular Simulation, 2007, 33, 287-304.	0.9	34
62	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
63	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
64	A molecular simulation study of the distribution of cation inÂzeolites. Adsorption, 2008, 14, 743-754.	1.4	32
65	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
66	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
67	Numerical Evidence of an Embryonic Orientational Phase Transition in Small Nitrogen Clusters. Physical Review Letters, 1996, 76, 4336-4339.	2.9	28
68	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
69	Structure and dynamics of simulated (SF6)N clusters in the size range N=7â€“55. Journal of Chemical Physics, 1993, 99, 9944-9953.	1.2	27
70	Thermodynamic study of water confinement in hydrophobic zeolites by Monte Carlo simulations. Molecular Simulation, 2009, 35, 24-30.	0.9	27
71	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
72	The temperature-size phase diagram of large SF6 clusters by computer simulation. Chemical Physics Letters, 1994, 218, 122-127.	1.2	26

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73	Flexibility and disorder in metalâ€“organic frameworks. Dalton Transactions, 2016, 45, 4058-4059.	1.6	26
74	Monte Carlo simulations of nanoconfined n-decane films. Physical Chemistry Chemical Physics, 1999, 1, 4083.	1.3	25
75	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
76	Placement of cations in NaX faujasite-type zeolite using (N,V,T) Monte Carlo simulations. Chemical Communications, 2001, , 2200-2201.	2.2	25
77	Fluid phase transitions at chemically heterogeneous, nonplanar solid substrates: Surface versus confinement effects. Journal of Chemical Physics, 2003, 118, 1453-1465.	1.2	25
78	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
79	Structure, Dynamics, and Thermodynamics of Intruded Electrolytes in ZIF-8. Journal of Physical Chemistry C, 2019, 123, 15589-15598.	1.5	22
80	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
81	Direct calculation of bubble points for alkane mixtures by molecular simulation. Molecular Physics, 2001, 99, 1423-1434.	0.8	20
82	Softening upon Adsorption in Microporous Materials: A Counterintuitive Mechanical Response. Journal of Physical Chemistry Letters, 2015, 6, 4265-4269.	2.1	20
83	Heat capacity of benzil near its phase transition. Journal of Chemical Physics, 1977, 67, 1789-1790.	1.2	19
84	Identification of aromatic molecules in intermediate boiling crude oil fractions by 2D n.m.r. spectroscopy. Fuel, 1991, 70, 641-646.	3.4	19
85	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
86	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
87	Is There a Vacancy-Induced Premelting in a Molecular Crystal?. Europhysics Letters, 1992, 18, 245-250.	0.7	16
88	Molecular dynamics study of the phase transitions in sulfur hexafluoride clusters of various size. The Journal of Physical Chemistry, 1993, 97, 10472-10477.	2.9	16
89	Monte Carlo simulations of squalane in the Gibbs ensemble. Fluid Phase Equilibria, 1999, 155, 167-176.	1.4	16
90	Melting curve and pressure-volume-temperature data of liquid dimethyl sulfoxide up to 150 MPa. Journal of Chemical & Engineering Data, 1980, 25, 206-208.	1.0	15

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91	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
92	Open questions on water confined in nanoporous materials. Communications Chemistry, 2021, 4, .	2.0	15
93	Structure of ultra-thin confined alkane films from Monte Carlo simulations. Molecular Physics, 2002, 100, 2109-2119.	0.8	14
94	Adsorption of Water and Aromatics in Faujasite Zeolites: A Molecular Simulation Study. Adsorption, 2005, 11, 279-282.	1.4	14
95	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
96	Adsorption deformation of microporous composites. Dalton Transactions, 2016, 45, 4136-4140.	1.6	14
97	Melting of sulfur hexafluoride clusters by molecular dynamics simulation. Molecular Physics, 1992, 76, 1079-1091.	0.8	12
98	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
99	Fluids confined by nanopatterned substrates of low symmetry. Molecular Physics, 2002, 100, 2971-2982.	0.8	11
100	Adsorption of Various Hydrocarbons in Siliceous Zeolites: A Molecular Simulation Study. Adsorption, 2005, 11, 379-382.	1.4	11
101	Molecularâ€dynamics investigation of surfaceâ€induced melting in sulfur hexafluoride. Journal of Chemical Physics, 1993, 98, 3290-3299.	1.2	9
102	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
103	Glassy Crystals VI. Nitrogen-14 Quadrupole Resonance in Glassy Crystalline Thiazole. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1986, 41, 348-352.	0.7	8
104	Determination of average molecular weights of high-boiling aromatic oil fractions by 13C and 1H nuclear magnetic resonance. Fuel, 1989, 68, 1158-1161.	3.4	8
105	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
106	Adsorption of Linear Alkanes in Zeolite Ferrierite from Molecular Simulations. Molecular Simulation, 2004, 30, 593-599.	0.9	8
107	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
108	The Melting Phase Transition in Small Carbon Dioxide Clusters. Molecular Simulation, 1997, 19, 285-299.	0.9	6

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109	Adsorption of n-Alkanes in Faujasite Zeolites: Molecular Simulation Study and Experimental Measurements. Adsorption Science and Technology, 2006, 24, 713-735.	1.5	6
110	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
111	The Sites of Premelting in Organic Compounds. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1991, 46, 917-919.	0.7	5
112	Nanoscopic liquid bridges exposed to a torsional strain. Physical Review E, 2003, 68, 066103.	0.8	5
113	Torsion-induced phase transitions in fluids confined between chemically decorated substrates. Journal of Chemical Physics, 2004, 121, 9077-9086.	1.2	5
114	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
115			