Benoit Coasne

List of Publications by Year
in descending order

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120 papers	5,930 citations	53794 45 h-index	76900 74 g-index
122 all docs	122 docs citations	122 times ranked	5920 citing authors

#	Article	IF	Citations
1	Effects of confinement on freezing and melting. Journal of Physics Condensed Matter, 2006, 18, R15-R68.	1.8	614
2	Realistic molecular model of kerogenâ€™s nanostructure. Nature Materials, 2016, 15, 576-582.	27.5	300
3	Structureâ€“property relationships of water adsorption in metalâ€“organic frameworks. New Journal of Chemistry, 2014, 38, 3102-3111.	2.8	252
4	Subcontinuum mass transport of condensed hydrocarbons in nanoporous media. Nature Communications, 2015, 6, 6949.	12.8	239
5	Validity of the t-plot Method to Assess Microporosity in Hierarchical Micro/Mesoporous Materials. Langmuir, 2014, 30, 13266-13274.	3.5	232
6	Adsorption, intrusion and freezing in porous silica: the view from the nanoscale. Chemical Society Reviews, 2013, 42, 4141.	38.1	204
7	Adsorption of Carbon Dioxide, Methane, and Their Mixtures in Porous Carbons: Effect of Surface Chemistry, Water Content, and Pore Disorder. Langmuir, 2013, 29, 3328-3338.	3.5	149
8	Adsorption of Simple Gases in MCM-41 Materials:Â The Role of Surface Roughness. Langmuir, 2006, 22, 194-202.	3.5	129
9	Freezing of Water Confined at the Nanoscale. Physical Review Letters, 2012, 109, 035701.	7.8	125
10	Nanoscale capillary freezing of ionic liquids confined between metallic interfaces and the role of electronic screening. Nature Materials, 2017, 16, 634-639.	27.5	125
11	Pressure enhancement in carbon nanopores: a major confinement effect. Physical Chemistry Chemical Physics, 2011, 13, 17163-17170.	2.8	124
12	Molecular simulation of water confined in nanoporous silica. Journal of Physics Condensed Matter, 2010, 22, 284110.	1.8	111
13	Role of hydrogen bonding in hysteresis observed in sorption-induced swelling of soft nanoporous polymers. Nature Communications, 2018, 9, 3507.	12.8	101
14	Activated desorption at heterogeneous interfaces and long-time kinetics of hydrocarbon recovery from nanoporous media. Nature Communications, 2016, 7, 11890.	12.8	100
15	Loading-Controlled Stiffening in Nanoconfined Ionic Liquids. Journal of Physical Chemistry Letters, 2011, 2, 1150-1154.	4.6	98
16	Multiscale adsorption and transport in hierarchical porous materials. New Journal of Chemistry, 2016, 40, 4078-4094.	2.8	88
17	A Grand Canonical Monte Carlo Study of Adsorption and Capillary Phenomena in Nanopores of Various Morphologies and Topologies: Testing the BET and BJH Characterization Methods. Particle and Particle Systems Characterization, 2004, 21, 149-160.	2.3	85
18	An artificial primitive mimic of the Gramicidin-A channel. Nature Communications, 2014, 5, 4142.	12.8	85

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19	Adsorption of volatile organic compounds in pure silica CHA, â^—BEA, MFI and STT-type zeolites. Microporous and Mesoporous Materials, 2013, 173, 147-154.	4.4	74
20	Free Volume Theory of Hydrocarbon Mixture Transport in Nanoporous Materials. Journal of Physical Chemistry Letters, 2016, 7, 3712-3717.	4.6	74
21	Specific Surface Area Determination for Microporous/Mesoporous Materials: The Case of Mesoporous FAU-Y Zeolites. Langmuir, 2018, 34, 14134-14142.	3.5	72
22	Ionic liquid confined in silica nanopores: molecular dynamics in the isobaricâ€“isothermal ensemble. Molecular Physics, 2014, 112, 1350-1361.	1.7	71
23	Effect of Chain Length and Pore Accessibility on Alkane Adsorption in Kerogen. Energy & Fuels, 2015, 29, 7889-7896.	5.1	65
24	Enhanced mechanical strength of zeolites by adsorption of guest molecules. Physical Chemistry Chemical Physics, 2011, 13, 20096.	2.8	64
25	Molecular Simulation of Adsorption and Transport in Hierarchical Porous Materials. Langmuir, 2013, 29, 7864-7875.	3.5	64
26	Simple Phenomenological Model for Phase Transitions in Confined Geometry. 2. Capillary Condensation/Evaporation in Cylindrical Mesopores. Langmuir, 2009, 25, 1393-1402.	3.5	62
27	Molecular Simulation of Nitrogen Adsorption in Nanoporous Silica. Langmuir, 2010, 26, 10872-10881.	3.5	61
28	Atomic-scale modelling of elastic and failure properties of clays. Molecular Physics, 2014, 112, 1294-1305.	1.7	61
29	Ion-specific adsorption and electroosmosis in charged amorphous porous silica. Physical Chemistry Chemical Physics, 2015, 17, 24683-24695.	2.8	60
30	Temperature Effect on Adsorption/Desorption Isotherms for a Simple Fluid Confined within Various Nanopores. Adsorption, 2005, 11, 289-294.	3.0	59
31	Probing Interconnectivity in Hierarchical Microporous/Mesoporous Materials Using Adsorption and Nuclear Magnetic Resonance Diffusion. Journal of Physical Chemistry C, 2016, 120, 1562-1569.	3.1	59
32	Domain theory for capillary condensation hysteresis. Physical Review B, 2005, 72, .	3.2	57
33	Effect of Morphological Defects on Gas Adsorption in Nanoporous Silicasâ€. Journal of Physical Chemistry C, 2007, 111, 15759-15770.	3.1	57
34	Capillary Condensation and Evaporation in Alumina Nanopores with Controlled Modulations. Langmuir, 2010, 26, 11894-11898.	3.5	57
35	Hydrophobic Transition in Porous Amorphous Silica. Journal of Physical Chemistry B, 2011, 115, 7881-7886.	2.6	57
36	On the molecular origin of high-pressure effects in nanoconfinement: The role of surface chemistry and roughness. Journal of Chemical Physics, 2013, 139, 144701.	3.0	57

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37	Adsorption, structure and dynamics of benzene in ordered and disordered porous carbons. Physical Chemistry Chemical Physics, 2011, 13, 3748-3757.	2.8	55
38	Structure and Dynamics of Benzene Confined in Silica Nanopores. Journal of Physical Chemistry C, 2011, 115, 15471-15479.	3.1	53
39	Solubility of Gases in Water Confined in Nanoporous Materials: ZSM-5, MCM-41, and MIL-100. Journal of Physical Chemistry C, 2015, 119, 21547-21554.	3.1	53
40	Effect of Pressure on the Freezing of Pure Fluids and Mixtures Confined in Nanopores. Journal of Physical Chemistry B, 2009, 113, 13874-13881.	2.6	52
41	Under pressure: Quasi-high pressure effects in nanopores. Microporous and Mesoporous Materials, 2012, 154, 19-23.	4.4	49
42	Molecular modeling of freezing of simple fluids confined within carbon nanotubes. Journal of Chemical Physics, 2005, 122, 144706.	3.0	48
43	Gas Uptake in Solvents Confined in Mesopores: Adsorption versus Enhanced Solubility. Journal of Physical Chemistry Letters, 2013, 4, 2274-2278.	4.6	48
44	Structure and Dynamics of an Electrolyte Confined in Charged Nanopores. Journal of Physical Chemistry C, 2014, 118, 5061-5072.	3.1	48
45	Atomistic Model of Micelle-Templated Mesoporous Silicas: Structural, Morphological, and Adsorption Properties. Langmuir, 2012, 28, 11131-11141.	3.5	47
46	Freezing of argon in ordered and disordered porous carbon. Physical Review B, 2007, 76, .	3.2	46
47	Enhanced H₂ Uptake in Solvents Confined in Mesoporous Metalâ€“Organic Framework. Journal of the American Chemical Society, 2012, 134, 17369-17371.	13.7	41
48	Bottom-up model of adsorption and transport in multiscale porous media. Physical Review E, 2015, 91, 032133.	2.1	39
49	Molecular Simulation of Ion-Specific Effects in Confined Electrolyte Solutions Using Polarizable Forcefields. Journal of Physical Chemistry C, 2010, 114, 12245-12257.	3.1	37
50	From Ionogels to Biredox Ionic Liquids: Some Emerging Opportunities for Electrochemical Energy Storage and Conversion Devices. Advanced Energy Materials, 2017, 7, 1700883.	19.5	36
51	Freezing and melting of azeotropic mixtures confined in nanopores: experiment and molecular simulation. Molecular Physics, 2005, 103, 3103-3113.	1.7	34
52	Reminiscent capillarity in subnanopores. Nature Communications, 2019, 10, 4642.	12.8	33
53	Freezing of Fluids Confined in a Disordered Nanoporous Structure. Physical Review Letters, 2006, 97, 105702.	7.8	32
54	Freezing of Mixtures Confined in a Slit Nanopore. Adsorption, 2005, 11, 301-306.	3.0	31

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55	Freezing and melting of binary mixtures confined in a nanopore. Molecular Physics, 2004, 102, 2149-2163.	1.7	30
56	Role of Silver Nanoparticles in Enhanced Xenon Adsorption Using Silver-Loaded Zeolites. Journal of Physical Chemistry C, 2014, 118, 25032-25040.	3.1	30
57	Poroelastic Theory Applied to the Adsorption-Induced Deformation of Vitreous Silica. Journal of Physical Chemistry B, 2014, 118, 14519-14525.	2.6	27
58	Characterization of hierarchical zeolites: Combining adsorption/intrusion, electron microscopy, diffraction and spectroscopic techniques. Microporous and Mesoporous Materials, 2019, 287, 167-176.	4.4	27
59	Adsorption and Dynamics in Hierarchical Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2014, 118, 7423-7433.	3.1	25
60	Pressure effects in confined nanophases. Molecular Simulation, 2014, 40, 721-730.	2.0	25
61	Intrusion and Retraction of Fluids in Nanopores: Effect of Morphological Heterogeneity. Journal of Physical Chemistry C, 2009, 113, 1953-1962.	3.1	24
62	Mechanism of H₂O Insertion and Chemical Bond Formation in AlPO₄-54Â·xH₂O at High Pressure. Journal of the American Chemical Society, 2015, 137, 584-587.	13.7	24
63	Optimized molecular reconstruction procedure combining hybrid reverse Monte Carlo and molecular dynamics. Journal of Chemical Physics, 2015, 142, 114112.	3.0	24
64	Molecular Simulation of the Phase Diagram of Methane Hydrate: Free Energy Calculations, Direct Coexistence Method, and Hyperparallel Tempering. Langmuir, 2017, 33, 11217-11230.	3.5	24
65	Reduced phase stability and faster formation/dissociation kinetics in confined methane hydrate. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	24
66	Gas oversolubility in nanoconfined liquids: Review and perspectives for adsorbent design. Microporous and Mesoporous Materials, 2019, 288, 109561.	4.4	23
67	Evaluation Methods of Adsorbents for Air Purification and Gas Separation at Low Concentration: Case Studies on Xenon and Krypton. Industrial & Engineering Chemistry Research, 2019, 58, 4560-4571.	3.7	23
68	On the Gibbsâ€“Thomson equation for the crystallization of confined fluids. Journal of Chemical Physics, 2021, 154, 114711.	3.0	22
69	Electronic screening using a virtual Thomasâ€“Fermi fluid for predicting wetting and phase transitions of ionic liquids at metal surfaces. Nature Materials, 2022, 21, 237-245.	27.5	22
70	Alkali Metal Cations Influence the CO₂ Adsorption Capacity of Nanosized Chabazite: Modeling vs Experiment. ACS Applied Nano Materials, 2022, 5, 5578-5588.	5.0	22
71	Water self-diffusion at the surface of silica glasses: effect of hydrophilic to hydrophobic transition. Molecular Physics, 2013, 111, 3410-3417.	1.7	21
72	Molecular intermittent dynamics of interfacial water: probing adsorption and bulk confinement. Soft Matter, 2013, 9, 8654.	2.7	20

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73	Woodâ€“Moisture Relationships Studied with Molecular Simulations: Methodological Guidelines. Forests, 2019, 10, 628.	2.1	19
74	Coupling of sorption and deformation in soft nanoporous polymers: Molecular simulation and poromechanics. Journal of the Mechanics and Physics of Solids, 2020, 137, 103830.	4.8	18
75	Bridging scales in disordered porous media by mapping molecular dynamics onto intermittent Brownian motion. Nature Communications, 2021, 12, 1043.	12.8	18
76	Hygromechanical mechanisms of wood cell wall revealed by molecular modeling and mixture rule analysis. Science Advances, 2021, 7, eabi8919.	10.3	18
77	Effect of Confinement on Freezing of CCl4 in Cylindrical Pores. Adsorption, 2005, 11, 391-396.	3.0	17
78	Role of Interfaces in Elasticity and Failure of Clayâ€“Organic Nanocomposites: Toughening upon Interface Weakening?. Langmuir, 2017, 33, 11457-11466.	3.5	17
79	Electrostatic interactions between ions near Thomasâ€“Fermi substrates and the surface energy of ionic crystals at imperfect metals. Faraday Discussions, 2017, 199, 129-158.	3.2	16
80	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.	3.5	15
81	Predicting Adsorption on Bare and Modified Silica Surfaces. Journal of Physical Chemistry C, 2015, 119, 6009-6017.	3.1	15
82	Adsorption in heterogeneous porous media: Hierarchical and composite solids. Microporous and Mesoporous Materials, 2016, 229, 145-154.	4.4	15
83	Revelation on the Complex Nature of Mesoporous Hierarchical FAU-Y Zeolites. Langmuir, 2018, 34, 11414-11423.	3.5	14
84	Molecular Simulation of Sorption-Induced Deformation in Atomistic Nanoporous Materials. Langmuir, 2019, 35, 7751-7758.	3.5	14
85	Moisture-induced crossover in the thermodynamic and mechanical response of hydrophilic biopolymer. Cellulose, 2020, 27, 89-99.	4.9	13
86	Probing the concept of line tension down to the nanoscale. Journal of Chemical Physics, 2020, 152, 094707.	3.0	12
87	Saturation of the Siliceous Zeolite TON with Neon at High Pressure. Journal of Physical Chemistry C, 2018, 122, 8455-8460.	3.1	11
88	Impact of Fluorocarbon Gaseous Environments on the Permeability of Foam Films to Air. Langmuir, 2020, 36, 13236-13243.	3.5	10
89	Interplay of Structure and Dynamics in Lithium/Ionic Liquid Electrolytes: Experiment and Molecular Simulation. Journal of Physical Chemistry B, 2021, 125, 1618-1631.	2.6	10
90	Organicâ€“Clay Interfacial Chemical Bonds Probed by ab Initio Calculations. Journal of Physical Chemistry C, 2015, 119, 6511-6517.	3.1	9

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91	Toward in Situ Measurement of the Density of Liquid Benzene Using Optical Kerr Effect Spectroscopy. Journal of Physical Chemistry B, 2016, 120, 9103-9114.	2.6	9
92	Enhanced H₂ Uptake of n-Alkanes Confined in Mesoporous Materials. Journal of Physical Chemistry C, 2014, 118, 10720-10727.	3.1	8
93	Assessing Polarizability Models for the Simulation of Low-Frequency Raman Spectra of Benzene. Journal of Physical Chemistry B, 2015, 119, 9345-9358.	2.6	8
94	Empirical Analysis of Optical Kerr Effect Spectra: A Case for Constraint. Journal of Physical Chemistry B, 2017, 121, 11376-11382.	2.6	8
95	Insertion and Confinement of H₂O in Hydrophobic Siliceous Zeolites at High Pressure. Journal of Physical Chemistry C, 2019, 123, 17432-17439.	3.1	8
96	A Poromechanical Model for Sorption Hysteresis in Nanoporous Polymers. Journal of Physical Chemistry B, 2020, 124, 8690-8703.	2.6	8
97	Disentangling Heat and Moisture Effects on Biopolymer Mechanics. Macromolecules, 2020, 53, 1527-1535.	4.8	8
98	The Pivotal Role of Critical Hydroxyl Concentration in Si-Rich Zeolites for Switching Vapor Adsorption. Journal of Physical Chemistry C, 2021, 125, 22890-22897.	3.1	8
99	Gas Adsorption in Zeolite and Thin Zeolite Layers: Molecular Simulation, Experiment, and Adsorption Potential Theory. Langmuir, 2022, 38, 5428-5438.	3.5	8
100	Adsorption-based characterization of hierarchical metalâ€“organic frameworks. Adsorption, 2014, 20, 349-357.	3.0	7
101	Surface Protolysis and Its Kinetics Impact the Electrical Double Layer. Physical Review Letters, 2022, 128, 056001.	7.8	7
102	Effect of Chlorine-Containing VOCs on Silver Migration and Sintering in ZSM-5 Used in a TSA Process. Catalysts, 2019, 9, 686.	3.5	6
103	Dispersion truncation affects the phase behavior of bulk and confined fluids: Coexistence, adsorption, and criticality. Journal of Chemical Physics, 2019, 150, 154104.	3.0	6
104	Role of cellulose nanocrystals on hysteretic sorption and deformation of nanocomposites. Cellulose, 2020, 27, 6945-6960.	4.9	6
105	Different Water Networks Confined in Unidirectional Hydrophilic Nanopores and Transitions with Temperature. Journal of Physical Chemistry C, 2021, 125, 14378-14393.	3.1	6
106	Comparison between Adsorption in Pores of a Simple Geometry and Realistic Models of Porous Materials. Materials Research Society Symposia Proceedings, 2003, 790, 1.	0.1	5
107	Effect of Surface Texture on Freezing in Nanopores: Surface-Induced versus Homogeneous Crystallization. Langmuir, 2015, 31, 2706-2713.	3.5	5
108	Lattice Boltzmann method for adsorption under stationary and transient conditions: Interplay between transport and adsorption kinetics in porous media. Physical Review E, 2021, 104, 015314.	2.1	5

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109	Carbon dioxide as a line active agent: Its impact on line tension and nucleation rate. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	5
110	High-Pressure Insertion of Dense H2 into a Model Zeolite. Journal of Physical Chemistry C, 2021, 125, 7511-7517.	3.1	4
111	Unexpected Orderâ€“Disorder Transition in Diacetylene Alcohol Langmuir Films. Langmuir, 2021, 37, 9034-9042.	3.5	4
112	Adsorption on alumina nanopores with conical shape. Nanoscale, 2018, 10, 18300-18305.	5.6	3
113	Cooperative Effects Dominating the Thermodynamics and Kinetics of Surfactant Adsorption in Porous Media: From Lateral Interactions to Surface Aggregation. Journal of Physical Chemistry B, 2020, 124, 10841-10849.	2.6	3
114	Heterogeneous Microscopic Dynamics of Intruded Water in a Superhydrophobic Nanoconfinement: Neutron Scattering and Molecular Modeling. Journal of Physical Chemistry B, 2021, 125, 10392-10399.	2.6	3
115	Morphology and topology assessment in hierarchical zeolite materials: adsorption hysteresis, scanning behavior, and domain theory. Inorganic Chemistry Frontiers, 2022, 9, 2903-2916.	6.0	3
116	Impact of adsorption kinetics on pollutant dispersion in water flowing in nanopores: A Lattice Boltzmann approach to stationary and transient conditions. Advances in Water Resources, 2022, 162, 104143.	3.8	2
117	Xylene Selectivity at the External Surface of Hierarchical Zeolites: Experiment and Molecular Modeling. Industrial & Engineering Chemistry Research, 2022, 61, 10184-10194.	3.7	2
118	Atomic-Spring-like Effect in Glassy Silica-Helium Composites. Journal of Physical Chemistry C, 2022, 126, 5722-5727.	3.1	1
119	Contribution of molecular simulation to the characterization of porous low-k materials. , 2015, , .		0
120	Insertion of Oxygen and Nitrogen in the Siliceous Zeolite TON at High Pressure. Journal of Physical Chemistry C, 2021, 125, 19517-19524.	3.1	0