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	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
2	Surface Protolysis and Its Kinetics Impact the Electrical Double Layer. Physical Review Letters, 2022, 128, 056001.	7.8	7
3	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
4	Atomic-Spring-like Effect in Glassy Silica-Helium Composites. Journal of Physical Chemistry C, 2022, 126, 5722-5727.	3.1	1
5	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
6	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
7	Gas Adsorption in Zeolite and Thin Zeolite Layers: Molecular Simulation, Experiment, and Adsorption Potential Theory. Langmuir, 2022, 38, 5428-5438.	3.5	8
8	Xylene Selectivity at the External Surface of Hierarchical Zeolites: Experiment and Molecular Modeling. Industrial & Engineering Chemistry Research, 2022, 61, 10184-10194.	3.7	2
9	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
10	Bridging scales in disordered porous media by mapping molecular dynamics onto intermittent Brownian motion. Nature Communications, 2021, 12, 1043.	12.8	18
11	On the Gibbsâ€“Thomson equation for the crystallization of confined fluids. Journal of Chemical Physics, 2021, 154, 114711.	3.0	22
12	High-Pressure Insertion of Dense H2 into a Model Zeolite. Journal of Physical Chemistry C, 2021, 125, 7511-7517.	3.1	4
13	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
14	Different Water Networks Confined in Unidirectional Hydrophilic Nanopores and Transitions with Temperature. Journal of Physical Chemistry C, 2021, 125, 14378-14393.	3.1	6
15	Unexpected Orderâ€“Disorder Transition in Diacetylene Alcohol Langmuir Films. Langmuir, 2021, 37, 9034-9042.	3.5	4
16	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
17	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
18	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

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19	Hygromechanical mechanisms of wood cell wall revealed by molecular modeling and mixture rule analysis. Science Advances, 2021, 7, eabi8919.	10.3	18
20	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
21	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
22	Moisture-induced crossover in the thermodynamic and mechanical response of hydrophilic biopolymer. Cellulose, 2020, 27, 89-99.	4.9	13
23	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
24	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
25	Impact of Fluorocarbon Gaseous Environments on the Permeability of Foam Films to Air. Langmuir, 2020, 36, 13236-13243.	3.5	10
26	A Poromechanical Model for Sorption Hysteresis in Nanoporous Polymers. Journal of Physical Chemistry B, 2020, 124, 8690-8703.	2.6	8
27	Role of cellulose nanocrystals on hysteretic sorption and deformation of nanocomposites. Cellulose, 2020, 27, 6945-6960.	4.9	6
28	Probing the concept of line tension down to the nanoscale. Journal of Chemical Physics, 2020, 152, 094707.	3.0	12
29	Disentangling Heat and Moisture Effects on Biopolymer Mechanics. Macromolecules, 2020, 53, 1527-1535.	4.8	8
30	Woodâ€“Moisture Relationships Studied with Molecular Simulations: Methodological Guidelines. Forests, 2019, 10, 628.	2.1	19
31	Reminiscent capillarity in subnanopores. Nature Communications, 2019, 10, 4642.	12.8	33
32	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
33	Gas oversolubility in nanoconfined liquids: Review and perspectives for adsorbent design. Microporous and Mesoporous Materials, 2019, 288, 109561.	4.4	23
34	Insertion and Confinement of H₂O in Hydrophobic Siliceous Zeolites at High Pressure. Journal of Physical Chemistry C, 2019, 123, 17432-17439.	3.1	8
35	Characterization of hierarchical zeolites: Combining adsorption/intrusion, electron microscopy, diffraction and spectroscopic techniques. Microporous and Mesoporous Materials, 2019, 287, 167-176.	4.4	27
36	Molecular Simulation of Sorption-Induced Deformation in Atomistic Nanoporous Materials. Langmuir, 2019, 35, 7751-7758.	3.5	14

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37	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
38	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
39	Saturation of the Siliceous Zeolite TON with Neon at High Pressure. Journal of Physical Chemistry C, 2018, 122, 8455-8460.	3.1	11
40	Adsorption on alumina nanopores with conical shape. Nanoscale, 2018, 10, 18300-18305.	5.6	3
41	Specific Surface Area Determination for Microporous/Mesoporous Materials: The Case of Mesoporous FAU-Y Zeolites. Langmuir, 2018, 34, 14134-14142.	3.5	72
42	Revelation on the Complex Nature of Mesoporous Hierarchical FAU-Y Zeolites. Langmuir, 2018, 34, 11414-11423.	3.5	14
43	Role of hydrogen bonding in hysteresis observed in sorption-induced swelling of soft nanoporous polymers. Nature Communications, 2018, 9, 3507.	12.8	101
44	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
45	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
46	Role of Interfaces in Elasticity and Failure of Clayâ€“Organic Nanocomposites: Toughening upon Interface Weakening?. Langmuir, 2017, 33, 11457-11466.	3.5	17
47	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
48	Empirical Analysis of Optical Kerr Effect Spectra: A Case for Constraint. Journal of Physical Chemistry B, 2017, 121, 11376-11382.	2.6	8
49	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
50	Adsorption in heterogeneous porous media: Hierarchical and composite solids. Microporous and Mesoporous Materials, 2016, 229, 145-154.	4.4	15
51	Free Volume Theory of Hydrocarbon Mixture Transport in Nanoporous Materials. Journal of Physical Chemistry Letters, 2016, 7, 3712-3717.	4.6	74
52	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
53	Activated desorption at heterogeneous interfaces and long-time kinetics of hydrocarbon recovery from nanoporous media. Nature Communications, 2016, 7, 11890.	12.8	100
54	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

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55	Multiscale adsorption and transport in hierarchical porous materials. New Journal of Chemistry, 2016, 40, 4078-4094.	2.8	88
56	Realistic molecular model of kerogenâ€™s nanostructure. Nature Materials, 2016, 15, 576-582.	27.5	300
57	Bottom-up model of adsorption and transport in multiscale porous media. Physical Review E, 2015, 91, 032133.	2.1	39
58	Contribution of molecular simulation to the characterization of porous low-k materials. , 2015, , .		0
59	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
60	Effect of Surface Texture on Freezing in Nanopores: Surface-Induced versus Homogeneous Crystallization. Langmuir, 2015, 31, 2706-2713.	3.5	5
61	Predicting Adsorption on Bare and Modified Silica Surfaces. Journal of Physical Chemistry C, 2015, 119, 6009-6017.	3.1	15
62	Subcontinuum mass transport of condensed hydrocarbons in nanoporous media. Nature Communications, 2015, 6, 6949.	12.8	239
63	Optimized molecular reconstruction procedure combining hybrid reverse Monte Carlo and molecular dynamics. Journal of Chemical Physics, 2015, 142, 114112.	3.0	24
64	Organicâ€“Clay Interfacial Chemical Bonds Probed by ab Initio Calculations. Journal of Physical Chemistry C, 2015, 119, 6511-6517.	3.1	9
65	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
66	Ion-specific adsorption and electroosmosis in charged amorphous porous silica. Physical Chemistry Chemical Physics, 2015, 17, 24683-24695.	2.8	60
67	Effect of Chain Length and Pore Accessibility on Alkane Adsorption in Kerogen. Energy & Fuels, 2015, 29, 7889-7896.	5.1	65
68	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
69	Poroelastic Theory Applied to the Adsorption-Induced Deformation of Vitreous Silica. Journal of Physical Chemistry B, 2014, 118, 14519-14525.	2.6	27
70	Validity of the t-plot Method to Assess Microporosity in Hierarchical Micro/Mesoporous Materials. Langmuir, 2014, 30, 13266-13274.	3.5	232
71	An artificial primitive mimic of the Gramicidin-A channel. Nature Communications, 2014, 5, 4142.	12.8	85
72	Adsorption-based characterization of hierarchical metalâ€“organic frameworks. Adsorption, 2014, 20, 349-357.	3.0	7

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73	Structure and Dynamics of an Electrolyte Confined in Charged Nanopores. Journal of Physical Chemistry C, 2014, 118, 5061-5072.	3.1	48
74	Adsorption and Dynamics in Hierarchical Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2014, 118, 7423-7433.	3.1	25
75	Atomic-scale modelling of elastic and failure properties of clays. Molecular Physics, 2014, 112, 1294-1305.	1.7	61
76	Structureâ€“property relationships of water adsorption in metalâ€“organic frameworks. New Journal of Chemistry, 2014, 38, 3102-3111.	2.8	252
77	Ionic liquid confined in silica nanopores: molecular dynamics in the isobaricâ€“isothermal ensemble. Molecular Physics, 2014, 112, 1350-1361.	1.7	71
78	Role of Silver Nanoparticles in Enhanced Xenon Adsorption Using Silver-Loaded Zeolites. Journal of Physical Chemistry C, 2014, 118, 25032-25040.	3.1	30
79	Enhanced H₂ Uptake of n-Alkanes Confined in Mesoporous Materials. Journal of Physical Chemistry C, 2014, 118, 10720-10727.	3.1	8
80	Pressure effects in confined nanophases. Molecular Simulation, 2014, 40, 721-730.	2.0	25
81	Molecular intermittent dynamics of interfacial water: probing adsorption and bulk confinement. Soft Matter, 2013, 9, 8654.	2.7	20
82	Water self-diffusion at the surface of silica glasses: effect of hydrophilic to hydrophobic transition. Molecular Physics, 2013, 111, 3410-3417.	1.7	21
83	Adsorption of volatile organic compounds in pure silica CHA, âˆ—BEA, MFI and STT-type zeolites. Microporous and Mesoporous Materials, 2013, 173, 147-154.	4.4	74
84	Adsorption, intrusion and freezing in porous silica: the view from the nanoscale. Chemical Society Reviews, 2013, 42, 4141.	38.1	204
85	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
86	Molecular Simulation of Adsorption and Transport in Hierarchical Porous Materials. Langmuir, 2013, 29, 7864-7875.	3.5	64
87	Gas Uptake in Solvents Confined in Mesopores: Adsorption versus Enhanced Solubility. Journal of Physical Chemistry Letters, 2013, 4, 2274-2278.	4.6	48
88	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
89	Freezing of Water Confined at the Nanoscale. Physical Review Letters, 2012, 109, 035701.	7.8	125
90	Enhanced H₂ Uptake in Solvents Confined in Mesoporous Metalâ€“Organic Framework. Journal of the American Chemical Society, 2012, 134, 17369-17371.	13.7	41

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91	Atomistic Model of Micelle-Templated Mesoporous Silicas: Structural, Morphological, and Adsorption Properties. Langmuir, 2012, 28, 11131-11141.	3.5	47
92	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
93	Under pressure: Quasi-high pressure effects in nanopores. Microporous and Mesoporous Materials, 2012, 154, 19-23.	4.4	49
94	Hydrophobic Transition in Porous Amorphous Silica. Journal of Physical Chemistry B, 2011, 115, 7881-7886.	2.6	57
95	Pressure enhancement in carbon nanopores: a major confinement effect. Physical Chemistry Chemical Physics, 2011, 13, 17163-17170.	2.8	124
96	Enhanced mechanical strength of zeolites by adsorption of guest molecules. Physical Chemistry Chemical Physics, 2011, 13, 20096.	2.8	64
97	Loading-Controlled Stiffening in Nanoconfined Ionic Liquids. Journal of Physical Chemistry Letters, 2011, 2, 1150-1154.	4.6	98
98	Adsorption, structure and dynamics of benzene in ordered and disordered porous carbons. Physical Chemistry Chemical Physics, 2011, 13, 3748-3757.	2.8	55
99	Structure and Dynamics of Benzene Confined in Silica Nanopores. Journal of Physical Chemistry C, 2011, 115, 15471-15479.	3.1	53
100	Molecular simulation of water confined in nanoporous silica. Journal of Physics Condensed Matter, 2010, 22, 284110.	1.8	111
101	Capillary Condensation and Evaporation in Alumina Nanopores with Controlled Modulations. Langmuir, 2010, 26, 11894-11898.	3.5	57
102	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
103	Molecular Simulation of Nitrogen Adsorption in Nanoporous Silica. Langmuir, 2010, 26, 10872-10881.	3.5	61
104	Intrusion and Retraction of Fluids in Nanopores: Effect of Morphological Heterogeneity. Journal of Physical Chemistry C, 2009, 113, 1953-1962.	3.1	24
105	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
106	Simple Phenomenological Model for Phase Transitions in Confined Geometry. 2. Capillary Condensation/Evaporation in Cylindrical Mesopores. Langmuir, 2009, 25, 1393-1402.	3.5	62
107	Freezing of argon in ordered and disordered porous carbon. Physical Review B, 2007, 76, .	3.2	46
108	Effect of Morphological Defects on Gas Adsorption in Nanoporous Silicasâ€. Journal of Physical Chemistry C, 2007, 111, 15759-15770.	3.1	57

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109	Adsorption of Simple Gases in MCM-41 Materials:Â The Role of Surface Roughness. Langmuir, 2006, 22, 194-202.	3.5	129
110	Effects of confinement on freezing and melting. Journal of Physics Condensed Matter, 2006, 18, R15-R68.	1.8	614
111	Freezing of Fluids Confined in a Disordered Nanoporous Structure. Physical Review Letters, 2006, 97, 105702.	7.8	32
112	Temperature Effect on Adsorption/Desorption Isotherms for a Simple Fluid Confined within Various Nanopores. Adsorption, 2005, 11, 289-294.	3.0	59
113	Freezing of Mixtures Confined in a Slit Nanopore. Adsorption, 2005, 11, 301-306.	3.0	31
114	Effect of Confinement on Freezing of CCl4 in Cylindrical Pores. Adsorption, 2005, 11, 391-396.	3.0	17
115	Domain theory for capillary condensation hysteresis. Physical Review B, 2005, 72, .	3.2	57
116	Molecular modeling of freezing of simple fluids confined within carbon nanotubes. Journal of Chemical Physics, 2005, 122, 144706.	3.0	48
117	Freezing and melting of azeotropic mixtures confined in nanopores: experiment and molecular simulation. Molecular Physics, 2005, 103, 3103-3113.	1.7	34
118	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
119	Freezing and melting of binary mixtures confined in a nanopore. Molecular Physics, 2004, 102, 2149-2163.	1.7	30
120	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