

Benoit Coasne

List of Publications by Year in descending order

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120
papers

5,930
citations

53660

45
h-index

76769

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. <i>Journal of Physics Condensed Matter</i> , 2006, 18, R15-R68.	0.7	614
2	Realistic molecular model of kerogen's nanostructure. <i>Nature Materials</i> , 2016, 15, 576-582.	13.3	300
3	Structure-property relationships of water adsorption in metal-organic frameworks. <i>New Journal of Chemistry</i> , 2014, 38, 3102-3111.	1.4	252
4	Subcontinuum mass transport of condensed hydrocarbons in nanoporous media. <i>Nature Communications</i> , 2015, 6, 6949.	5.8	239
5	Validity of the <i>t</i> -plot Method to Assess Microporosity in Hierarchical Micro/Mesoporous Materials. <i>Langmuir</i> , 2014, 30, 13266-13274.	1.6	232
6	Adsorption, intrusion and freezing in porous silica: the view from the nanoscale. <i>Chemical Society Reviews</i> , 2013, 42, 4141.	18.7	204
7	Adsorption of Carbon Dioxide, Methane, and Their Mixtures in Porous Carbons: Effect of Surface Chemistry, Water Content, and Pore Disorder. <i>Langmuir</i> , 2013, 29, 3328-3338.	1.6	149
8	Adsorption of Simple Gases in MCM-41 Materials: The Role of Surface Roughness. <i>Langmuir</i> , 2006, 22, 194-202.	1.6	129
9	Freezing of Water Confined at the Nanoscale. <i>Physical Review Letters</i> , 2012, 109, 035701.	2.9	125
10	Nanoscale capillary freezing of ionic liquids confined between metallic interfaces and the role of electronic screening. <i>Nature Materials</i> , 2017, 16, 634-639.	13.3	125
11	Pressure enhancement in carbon nanopores: a major confinement effect. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 17163-17170.	1.3	124
12	Molecular simulation of water confined in nanoporous silica. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 284110.	0.7	111
13	Role of hydrogen bonding in hysteresis observed in sorption-induced swelling of soft nanoporous polymers. <i>Nature Communications</i> , 2018, 9, 3507.	5.8	101
14	Activated desorption at heterogeneous interfaces and long-time kinetics of hydrocarbon recovery from nanoporous media. <i>Nature Communications</i> , 2016, 7, 11890.	5.8	100
15	Loading-Controlled Stiffening in Nanoconfined Ionic Liquids. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1150-1154.	2.1	98
16	Multiscale adsorption and transport in hierarchical porous materials. <i>New Journal of Chemistry</i> , 2016, 40, 4078-4094.	1.4	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. <i>Particle and Particle Systems Characterization</i> , 2004, 21, 149-160.	1.2	85
18	An artificial primitive mimic of the Gramicidin-A channel. <i>Nature Communications</i> , 2014, 5, 4142.	5.8	85

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19	Adsorption of volatile organic compounds in pure silica CHA, β -BEA, MFI and STT-type zeolites. <i>Microporous and Mesoporous Materials</i> , 2013, 173, 147-154.	2.2	74
20	Free Volume Theory of Hydrocarbon Mixture Transport in Nanoporous Materials. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3712-3717.	2.1	74
21	Specific Surface Area Determination for Microporous/Mesoporous Materials: The Case of Mesoporous FAU-Y Zeolites. <i>Langmuir</i> , 2018, 34, 14134-14142.	1.6	72
22	Ionic liquid confined in silica nanopores: molecular dynamics in the isobaric-isothermal ensemble. <i>Molecular Physics</i> , 2014, 112, 1350-1361.	0.8	71
23	Effect of Chain Length and Pore Accessibility on Alkane Adsorption in Kerogen. <i>Energy & Fuels</i> , 2015, 29, 7889-7896.	2.5	65
24	Enhanced mechanical strength of zeolites by adsorption of guest molecules. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20096.	1.3	64
25	Molecular Simulation of Adsorption and Transport in Hierarchical Porous Materials. <i>Langmuir</i> , 2013, 29, 7864-7875.	1.6	64
26	Simple Phenomenological Model for Phase Transitions in Confined Geometry. 2. Capillary Condensation/Evaporation in Cylindrical Mesopores. <i>Langmuir</i> , 2009, 25, 1393-1402.	1.6	62
27	Molecular Simulation of Nitrogen Adsorption in Nanoporous Silica. <i>Langmuir</i> , 2010, 26, 10872-10881.	1.6	61
28	Atomic-scale modelling of elastic and failure properties of clays. <i>Molecular Physics</i> , 2014, 112, 1294-1305.	0.8	61
29	Ion-specific adsorption and electroosmosis in charged amorphous porous silica. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 24683-24695.	1.3	60
30	Temperature Effect on Adsorption/Desorption Isotherms for a Simple Fluid Confined within Various Nanopores. <i>Adsorption</i> , 2005, 11, 289-294.	1.4	59
31	Probing Interconnectivity in Hierarchical Microporous/Mesoporous Materials Using Adsorption and Nuclear Magnetic Resonance Diffusion. <i>Journal of Physical Chemistry C</i> , 2016, 120, 1562-1569.	1.5	59
32	Domain theory for capillary condensation hysteresis. <i>Physical Review B</i> , 2005, 72, .	1.1	57
33	Effect of Morphological Defects on Gas Adsorption in Nanoporous Silicas. <i>Journal of Physical Chemistry C</i> , 2007, 111, 15759-15770.	1.5	57
34	Capillary Condensation and Evaporation in Alumina Nanopores with Controlled Modulations. <i>Langmuir</i> , 2010, 26, 11894-11898.	1.6	57
35	Hydrophobic Transition in Porous Amorphous Silica. <i>Journal of Physical Chemistry B</i> , 2011, 115, 7881-7886.	1.2	57
36	On the molecular origin of high-pressure effects in nanoconfinement: The role of surface chemistry and roughness. <i>Journal of Chemical Physics</i> , 2013, 139, 144701.	1.2	57

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37	Adsorption, structure and dynamics of benzene in ordered and disordered porous carbons. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 3748-3757.	1.3	55
38	Structure and Dynamics of Benzene Confined in Silica Nanopores. <i>Journal of Physical Chemistry C</i> , 2011, 115, 15471-15479.	1.5	53
39	Solubility of Gases in Water Confined in Nanoporous Materials: ZSM-5, MCM-41, and MIL-100. <i>Journal of Physical Chemistry C</i> , 2015, 119, 21547-21554.	1.5	53
40	Effect of Pressure on the Freezing of Pure Fluids and Mixtures Confined in Nanopores. <i>Journal of Physical Chemistry B</i> , 2009, 113, 13874-13881.	1.2	52
41	Under pressure: Quasi-high pressure effects in nanopores. <i>Microporous and Mesoporous Materials</i> , 2012, 154, 19-23.	2.2	49
42	Molecular modeling of freezing of simple fluids confined within carbon nanotubes. <i>Journal of Chemical Physics</i> , 2005, 122, 144706.	1.2	48
43	Gas Uptake in Solvents Confined in Mesopores: Adsorption versus Enhanced Solubility. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2274-2278.	2.1	48
44	Structure and Dynamics of an Electrolyte Confined in Charged Nanopores. <i>Journal of Physical Chemistry C</i> , 2014, 118, 5061-5072.	1.5	48
45	Atomistic Model of Micelle-Templated Mesoporous Silicas: Structural, Morphological, and Adsorption Properties. <i>Langmuir</i> , 2012, 28, 11131-11141.	1.6	47
46	Freezing of argon in ordered and disordered porous carbon. <i>Physical Review B</i> , 2007, 76, .	1.1	46
47	Enhanced H ₂ Uptake in Solvents Confined in Mesoporous Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2012, 134, 17369-17371.	6.6	41
48	Bottom-up model of adsorption and transport in multiscale porous media. <i>Physical Review E</i> , 2015, 91, 032133.	0.8	39
49	Molecular Simulation of Ion-Specific Effects in Confined Electrolyte Solutions Using Polarizable Forcefields. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12245-12257.	1.5	37
50	From Ionogels to Biredox Ionic Liquids: Some Emerging Opportunities for Electrochemical Energy Storage and Conversion Devices. <i>Advanced Energy Materials</i> , 2017, 7, 1700883.	10.2	36
51	Freezing and melting of azeotropic mixtures confined in nanopores: experiment and molecular simulation. <i>Molecular Physics</i> , 2005, 103, 3103-3113.	0.8	34
52	Reminiscent capillarity in subnanopores. <i>Nature Communications</i> , 2019, 10, 4642.	5.8	33
53	Freezing of Fluids Confined in a Disordered Nanoporous Structure. <i>Physical Review Letters</i> , 2006, 97, 105702.	2.9	32
54	Freezing of Mixtures Confined in a Slit Nanopore. <i>Adsorption</i> , 2005, 11, 301-306.	1.4	31

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55	Freezing and melting of binary mixtures confined in a nanopore. <i>Molecular Physics</i> , 2004, 102, 2149-2163.	0.8	30
56	Role of Silver Nanoparticles in Enhanced Xenon Adsorption Using Silver-Loaded Zeolites. <i>Journal of Physical Chemistry C</i> , 2014, 118, 25032-25040.	1.5	30
57	Poroelastic Theory Applied to the Adsorption-Induced Deformation of Vitreous Silica. <i>Journal of Physical Chemistry B</i> , 2014, 118, 14519-14525.	1.2	27
58	Characterization of hierarchical zeolites: Combining adsorption/intrusion, electron microscopy, diffraction and spectroscopic techniques. <i>Microporous and Mesoporous Materials</i> , 2019, 287, 167-176.	2.2	27
59	Adsorption and Dynamics in Hierarchical Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2014, 118, 7423-7433.	1.5	25
60	Pressure effects in confined nanophases. <i>Molecular Simulation</i> , 2014, 40, 721-730.	0.9	25
61	Intrusion and Retraction of Fluids in Nanopores: Effect of Morphological Heterogeneity. <i>Journal of Physical Chemistry C</i> , 2009, 113, 1953-1962.	1.5	24
62	Mechanism of H ₂ O Insertion and Chemical Bond Formation in AlPO ₄ -54 Å ^x H ₂ O at High Pressure. <i>Journal of the American Chemical Society</i> , 2015, 137, 584-587.	6.6	24
63	Optimized molecular reconstruction procedure combining hybrid reverse Monte Carlo and molecular dynamics. <i>Journal of Chemical Physics</i> , 2015, 142, 114112.	1.2	24
64	Molecular Simulation of the Phase Diagram of Methane Hydrate: Free Energy Calculations, Direct Coexistence Method, and Hyperparallel Tempering. <i>Langmuir</i> , 2017, 33, 11217-11230.	1.6	24
65	Reduced phase stability and faster formation/dissociation kinetics in confined methane hydrate. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	24
66	Gas oversolubility in nanoconfined liquids: Review and perspectives for adsorbent design. <i>Microporous and Mesoporous Materials</i> , 2019, 288, 109561.	2.2	23
67	Evaluation Methods of Adsorbents for Air Purification and Gas Separation at Low Concentration: Case Studies on Xenon and Krypton. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 4560-4571.	1.8	23
68	On the Gibbs-Thomson equation for the crystallization of confined fluids. <i>Journal of Chemical Physics</i> , 2021, 154, 114711.	1.2	22
69	Electronic screening using a virtual Thomas-Fermi fluid for predicting wetting and phase transitions of ionic liquids at metal surfaces. <i>Nature Materials</i> , 2022, 21, 237-245.	13.3	22
70	Alkali Metal Cations Influence the CO ₂ Adsorption Capacity of Nanosized Chabazite: Modeling vs Experiment. <i>ACS Applied Nano Materials</i> , 2022, 5, 5578-5588.	2.4	22
71	Water self-diffusion at the surface of silica glasses: effect of hydrophilic to hydrophobic transition. <i>Molecular Physics</i> , 2013, 111, 3410-3417.	0.8	21
72	Molecular intermittent dynamics of interfacial water: probing adsorption and bulk confinement. <i>Soft Matter</i> , 2013, 9, 8654.	1.2	20

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73	Wood's Moisture Relationships Studied with Molecular Simulations: Methodological Guidelines. <i>Forests</i> , 2019, 10, 628.	0.9	19
74	Coupling of sorption and deformation in soft nanoporous polymers: Molecular simulation and poromechanics. <i>Journal of the Mechanics and Physics of Solids</i> , 2020, 137, 103830.	2.3	18
75	Bridging scales in disordered porous media by mapping molecular dynamics onto intermittent Brownian motion. <i>Nature Communications</i> , 2021, 12, 1043.	5.8	18
76	Hygromechanical mechanisms of wood cell wall revealed by molecular modeling and mixture rule analysis. <i>Science Advances</i> , 2021, 7, eabi8919.	4.7	18
77	Effect of Confinement on Freezing of CCl ₄ in Cylindrical Pores. <i>Adsorption</i> , 2005, 11, 391-396.	1.4	17
78	Role of Interfaces in Elasticity and Failure of Clay/Organic Nanocomposites: Toughening upon Interface Weakening?. <i>Langmuir</i> , 2017, 33, 11457-11466.	1.6	17
79	Electrostatic interactions between ions near Thomas-Fermi substrates and the surface energy of ionic crystals at imperfect metals. <i>Faraday Discussions</i> , 2017, 199, 129-158.	1.6	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. <i>Langmuir</i> , 2012, 28, 9526-9534.	1.6	15
81	Predicting Adsorption on Bare and Modified Silica Surfaces. <i>Journal of Physical Chemistry C</i> , 2015, 119, 6009-6017.	1.5	15
82	Adsorption in heterogeneous porous media: Hierarchical and composite solids. <i>Microporous and Mesoporous Materials</i> , 2016, 229, 145-154.	2.2	15
83	Revelation on the Complex Nature of Mesoporous Hierarchical FAU-Y Zeolites. <i>Langmuir</i> , 2018, 34, 11414-11423.	1.6	14
84	Molecular Simulation of Sorption-Induced Deformation in Atomistic Nanoporous Materials. <i>Langmuir</i> , 2019, 35, 7751-7758.	1.6	14
85	Moisture-induced crossover in the thermodynamic and mechanical response of hydrophilic biopolymer. <i>Cellulose</i> , 2020, 27, 89-99.	2.4	13
86	Probing the concept of line tension down to the nanoscale. <i>Journal of Chemical Physics</i> , 2020, 152, 094707.	1.2	12
87	Saturation of the Siliceous Zeolite TON with Neon at High Pressure. <i>Journal of Physical Chemistry C</i> , 2018, 122, 8455-8460.	1.5	11
88	Impact of Fluorocarbon Gaseous Environments on the Permeability of Foam Films to Air. <i>Langmuir</i> , 2020, 36, 13236-13243.	1.6	10
89	Interplay of Structure and Dynamics in Lithium/Ionic Liquid Electrolytes: Experiment and Molecular Simulation. <i>Journal of Physical Chemistry B</i> , 2021, 125, 1618-1631.	1.2	10
90	Organic/Clay Interfacial Chemical Bonds Probed by ab Initio Calculations. <i>Journal of Physical Chemistry C</i> , 2015, 119, 6511-6517.	1.5	9

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91	Toward in Situ Measurement of the Density of Liquid Benzene Using Optical Kerr Effect Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9103-9114.	1.2	9
92	Enhanced H ₂ Uptake of <i>n</i> -Alkanes Confined in Mesoporous Materials. <i>Journal of Physical Chemistry C</i> , 2014, 118, 10720-10727.	1.5	8
93	Assessing Polarizability Models for the Simulation of Low-Frequency Raman Spectra of Benzene. <i>Journal of Physical Chemistry B</i> , 2015, 119, 9345-9358.	1.2	8
94	Empirical Analysis of Optical Kerr Effect Spectra: A Case for Constraint. <i>Journal of Physical Chemistry B</i> , 2017, 121, 11376-11382.	1.2	8
95	Insertion and Confinement of H ₂ O in Hydrophobic Siliceous Zeolites at High Pressure. <i>Journal of Physical Chemistry C</i> , 2019, 123, 17432-17439.	1.5	8
96	A Poromechanical Model for Sorption Hysteresis in Nanoporous Polymers. <i>Journal of Physical Chemistry B</i> , 2020, 124, 8690-8703.	1.2	8
97	Disentangling Heat and Moisture Effects on Biopolymer Mechanics. <i>Macromolecules</i> , 2020, 53, 1527-1535.	2.2	8
98	The Pivotal Role of Critical Hydroxyl Concentration in Si-Rich Zeolites for Switching Vapor Adsorption. <i>Journal of Physical Chemistry C</i> , 2021, 125, 22890-22897.	1.5	8
99	Gas Adsorption in Zeolite and Thin Zeolite Layers: Molecular Simulation, Experiment, and Adsorption Potential Theory. <i>Langmuir</i> , 2022, 38, 5428-5438.	1.6	8
100	Adsorption-based characterization of hierarchical metal-organic frameworks. <i>Adsorption</i> , 2014, 20, 349-357.	1.4	7
101	Surface Protolysis and Its Kinetics Impact the Electrical Double Layer. <i>Physical Review Letters</i> , 2022, 128, 056001.	2.9	7
102	Effect of Chlorine-Containing VOCs on Silver Migration and Sintering in ZSM-5 Used in a TSA Process. <i>Catalysts</i> , 2019, 9, 686.	1.6	6
103	Dispersion truncation affects the phase behavior of bulk and confined fluids: Coexistence, adsorption, and criticality. <i>Journal of Chemical Physics</i> , 2019, 150, 154104.	1.2	6
104	Role of cellulose nanocrystals on hysteretic sorption and deformation of nanocomposites. <i>Cellulose</i> , 2020, 27, 6945-6960.	2.4	6
105	Different Water Networks Confined in Unidirectional Hydrophilic Nanopores and Transitions with Temperature. <i>Journal of Physical Chemistry C</i> , 2021, 125, 14378-14393.	1.5	6
106	Comparison between Adsorption in Pores of a Simple Geometry and Realistic Models of Porous Materials. <i>Materials Research Society Symposia Proceedings</i> , 2003, 790, 1.	0.1	5
107	Effect of Surface Texture on Freezing in Nanopores: Surface-Induced versus Homogeneous Crystallization. <i>Langmuir</i> , 2015, 31, 2706-2713.	1.6	5
108	Lattice Boltzmann method for adsorption under stationary and transient conditions: Interplay between transport and adsorption kinetics in porous media. <i>Physical Review E</i> , 2021, 104, 015314.	0.8	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, .	3.3	5
110	High-Pressure Insertion of Dense H2 into a Model Zeolite. Journal of Physical Chemistry C, 2021, 125, 7511-7517.	1.5	4
111	Unexpected Order-Disorder Transition in Diacetylene Alcohol Langmuir Films. Langmuir, 2021, 37, 9034-9042.	1.6	4
112	Adsorption on alumina nanopores with conical shape. Nanoscale, 2018, 10, 18300-18305.	2.8	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.	1.2	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.	1.2	3
115	Morphology and topology assessment in hierarchical zeolite materials: adsorption hysteresis, scanning behavior, and domain theory. Inorganic Chemistry Frontiers, 2022, 9, 2903-2916.	3.0	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.	1.7	2
117	Xylene Selectivity at the External Surface of Hierarchical Zeolites: Experiment and Molecular Modeling. Industrial & Engineering Chemistry Research, 2022, 61, 10184-10194.	1.8	2
118	Atomic-Spring-like Effect in Glassy Silica-Helium Composites. Journal of Physical Chemistry C, 2022, 126, 5722-5727.	1.5	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.	1.5	0