Bernard Rousseau

List of Publications by Year
in descending order

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92 papers	3,229 citations	109321 35 h-index	161849 54 g-index
95 all docs	95 docs citations	95 times ranked	2459 citing authors

#	Article	IF	Citations
1	Optimization of the anisotropic united atoms intermolecular potential forn-alkanes. Journal of Chemical Physics, 2000, 112, 5499-5510.	3.0	270
2	Flash Point and Cetane Number Predictions for Fuel Compounds Using Quantitative Structure Property Relationship (QSPR) Methods. Energy & Fuels, 2011, 25, 3900-3908.	5.1	121
3	A General Guidebook for the Theoretical Prediction of Physicochemical Properties of Chemicals for Regulatory Purposes. Chemical Reviews, 2015, 115, 13093-13164.	47.7	116
4	Soret and mass diffusion measurements and molecular dynamics simulations ofn-pentaneâ€“n-decane mixtures. Journal of Chemical Physics, 2002, 116, 3718-3729.	3.0	100
5	Self-diffusion of n-alkanes in silicalite using molecular dynamics simulation: A comparison between rigid and flexible frameworks. Physical Chemistry Chemical Physics, 2004, 6, 775.	2.8	100
6	Molecular simulation of the thermophysical properties of fluids: From understanding toward quantitative predictions. Journal of Molecular Liquids, 2007, 134, 71-89.	4.9	99
7	Molecular simulations of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-alkane liquid-vapor interface: Interfacial properties and their long range corrections. Physical Review E, 2007, 75, 051602.	2.1	97
8	Prediction of Density and Viscosity of Biofuel Compounds Using Machine Learning Methods. Energy & Fuels, 2012, 26, 2416-2426.	5.1	83
9	Microscopic Interpretation of a Pure Chemical Contribution to the Soret Effect. Physical Review Letters, 2007, 98, 125901.	7.8	74
10	Viscosity of the 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquid from equilibrium and nonequilibrium molecular dynamics. Physical Chemistry Chemical Physics, 2010, 12, 930-936.	2.8	74
11	Fluid transport properties by equilibrium molecular dynamics. III. Evaluation of united atom interaction potential models for pure alkanes. Journal of Chemical Physics, 2000, 112, 7581-7590.	3.0	72
12	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.	3.0	71
13	A Grand Canonical Monte Carlo study of argon adsorption/condensation in mesoporous silica glasses. Physical Chemistry Chemical Physics, 2001, 3, 1207-1212.	2.8	70
14	Onset of Entanglements Revisited. Dynamical Analysis. Macromolecules, 2009, 42, 7485-7494.	4.8	66
15	A New Model for Thermal Diffusion: Kinetic Approach. Journal of the American Chemical Society, 2008, 130, 10963-10969.	13.7	60
16	Transport properties of dimethyl sulfoxide aqueous solutions. Journal of Chemical Physics, 2003, 119, 4782-4789.	3.0	59
17	Prediction of Flash Points for Fuel Mixtures Using Machine Learning and a Novel Equation. Energy & Fuels, 2013, 27, 3811-3820.	5.1	56
18	Onset of Entanglements Revisited. Topological Analysis. Macromolecules, 2009, 42, 7474-7484.	4.8	53

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19	Dissipative particle dynamics simulations of polymer melts. I. Building potential of mean force for polyethylene and cis-polybutadiene. Journal of Chemical Physics, 2004, 121, 6538-6546.	3.0	52
20	Fluid transport properties by equilibrium molecular dynamics. I. Methodology at extreme fluid states. Journal of Chemical Physics, 1999, 110, 4047-4059.	3.0	50
21	Computing the Soret coefficient in aqueous mixtures using boundary driven nonequilibrium molecular dynamics. Journal of Chemical Physics, 2005, 122, 114503.	3.0	50
22	Dynamic and structural behavior of different rigid nonpolarizable models of water. Journal of Chemical Physics, 2003, 118, 7954-7964.	3.0	49
23	Conservative and dissipative force field for simulation of coarse-grained alkane molecules: A bottom-up approach. Journal of Chemical Physics, 2014, 140, 134113.	3.0	48
24	Influence of the adjustable parameters of the DPD on the global and local dynamics of a polymer melt. Polymer, 2007, 48, 3584-3592.	3.8	47
25	Rheology of model confined ultrathin fluid films. I. Statistical mechanics of the surface force apparatus experiments. Journal of Chemical Physics, 1997, 106, 7295-7302.	3.0	44
26	Optimization of the anisotropic united atoms intermolecular potential for n-alkanes: Improvement of transport properties. Journal of Chemical Physics, 2006, 125, 044517.	3.0	44
27	Fluid transport properties by equilibrium molecular dynamics. II. Multicomponent systems. Journal of Chemical Physics, 1999, 110, 4060-4067.	3.0	42
28	Impact of Thermodiffusion on the Initial Vertical Distribution of Species in Hydrocarbon Reservoirs. Microgravity Science and Technology, 2016, 28, 79-86.	1.4	42
29	Soret coefficient for liquid argon-krypton mixtures via equilibrium and nonequilibrium molecular dynamics: A comparison with experiments. Physical Review E, 2002, 66, 031201.	2.1	41
30	The role of molecular interactions in the change of sign of the Soret coefficient. Europhysics Letters, 2004, 67, 976-982.	2.0	40
31	Melting of Lennard-Jones clusters in confined geometries. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1996, 37, 49-53.	1.0	39
32	Thermal diffusion in simple liquid mixtures: what have we learnt from molecular dynamics simulations?. Molecular Physics, 2013, 111, 3394-3403.	1.7	38
33	On the rational formulation of alternative fuels: melting point and net heat of combustion predictions for fuel compounds using machine learning methods. SAR and QSAR in Environmental Research, 2013, 24, 259-277.	2.2	38
34	Thermal diffusion in alkane binary mixtures. Fluid Phase Equilibria, 1998, 150-151, 151-159.	2.5	37
35	Structure and solvation forces in confined alkane films. Physical Chemistry Chemical Physics, 2001, 3, 1155-1159.	2.8	37
36	Computation of elastic constants of solids using molecular simulation: comparison of constant volume and constant pressure ensemble methods. Molecular Simulation, 2017, 43, 1413-1422.	2.0	36

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37	Fluid in mineral interfacesâ€"molecular simulations of structure and diffusion. Geophysical Research Letters, 2002, 29, 13-1.	4.0	35
38	Molecular simulation applied to fluid properties in the oil and gas industry. Molecular Simulation, 2007, 33, 287-304.	2.0	34
39	Coarse-grained simulations of cis- and trans-polybutadiene: A bottom-up approach. Journal of Chemical Physics, 2017, 146, 074904.	3.0	34
40	Competition Reactions of H₂O^{â€¢+} Radical in Concentrated Cl^{â€“} Aqueous Solutions: Picosecond Pulse Radiolysis Study. Journal of Physical Chemistry A, 2012, 116, 11509-11518.	2.5	33
41	Thermodiffusion in multicomponent n-alkane mixtures. Npj Microgravity, 2017, 3, 20.	3.7	32
42	Molecular simulation of the solubility and diffusion of carbon dioxide and hydrogen sulfide in polyethylene melts. Fluid Phase Equilibria, 2007, 261, 168-175.	2.5	30
43	Classical Force Field for Hydrofluorocarbon Molecular Simulations. Application to the Study of Gas Solubility in Poly(vinylidene fluoride). Journal of Physical Chemistry A, 2015, 119, 140-151.	2.5	30
44	The temperature-size phase diagram of large SF6 clusters by computer simulation. Chemical Physics Letters, 1994, 218, 122-127.	2.6	26
45	Gas mixture solubilities in polyethylene below its melting temperature: Experimental and molecular simulation studies. Journal of Membrane Science, 2012, 390-391, 194-200.	8.2	26
46	Prediction of Fluid Mixture Transport Properties by Molecular Dynamics. International Journal of Thermophysics, 1998, 19, 437-448.	2.1	25
47	Monte Carlo simulations of nanoconfined n-decane films. Physical Chemistry Chemical Physics, 1999, 1, 4083.	2.8	25
48	Molecular simulations of the solubility of gases in polyethylene below its melting temperature. Polymer, 2010, 51, 4978-4984.	3.8	25
49	Interfacial tension in oilâ€"waterâ€"surfactant systems: On the role of intra-molecular forces on interfacial tension values using DPD simulations. Journal of Chemical Physics, 2013, 138, 144102.	3.0	25
50	Vaporâ€"liquid equilibrium and molecular simulation data for carbon dioxide (CO2)â€¯+â€¯trans-1,3,3,3-tetrafluoroprop-1-ene (R-1234ze(E)) mixture at temperatures from 283.32 to 353.02â€¯K and pressures up to 7.6â€¯MPa. International Journal of Refrigeration, 2019, 98, 362-371.	3.4	25
51	Optimisation of the dynamical behaviour of the anisotropic united atom model of branched alkanes: application to the molecular simulation of fuel gasoline. Molecular Simulation, 2008, 34, 211-230.	2.0	24
52	Influence of high pressures on CH4, CO2 and H2S solubility in polyethylene: Experimental and molecular simulation approaches for pure gas and gas mixtures. Modelling of the sorption isotherms. Journal of Membrane Science, 2015, 490, 380-388.	8.2	24
53	Solvation Force and Confinement-Induced Phase Transitions of Model Ultra Thin Films. Molecular Simulation, 1996, 17, 199-215.	2.0	23
54	Isotopic Soret effect in ternary mixtures: Theoretical predictions and molecular simulations. Journal of Chemical Physics, 2015, 143, 174503.	3.0	23

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55	Parameterization of a mesoscopic model for the self-assembly of linear sodium alkyl sulfates. Journal of Chemical Physics, 2014, 140, 204902.	3.0	22
56	Identification of aromatic molecules in intermediate boiling crude oil fractions by 2D n.m.r. spectroscopy. Fuel, 1991, 70, 641-646.	6.4	19
57	Limit of Miscibility and Nanophase Separation in Associated Mixtures. Journal of Physical Chemistry B, 2013, 117, 9718-9727.	2.6	19
58	Is There a Vacancy-Induced Premelting in a Molecular Crystal?. Europhysics Letters, 1992, 18, 245-250.	2.0	16
59	Structure of ultra-thin confined alkane films from Monte Carlo simulations. Molecular Physics, 2002, 100, 2109-2119.	1.7	14
60	Self-diffusion ofn-alkanes in MFI type Zeolite using Molecular Dynamics Simulations with an Anisotropic United Atom (AUA) Forcefield. Molecular Simulation, 2004, 30, 617-620.	2.0	13
61	Rational Formulation of Alternative Fuels using QSPR Methods: Application to Jet Fuels. Oil and Gas Science and Technology, 2013, 68, 651-662.	1.4	13
62	Scaling behaviour of different polymer models in dissipative particle dynamics of unentangled melts. Molecular Simulation, 2014, 40, 1274-1289.	2.0	13
63	Molecular simulation of the water-triolein-oleic acid mixture: Local structure and thermodynamic properties. Journal of Chemical Physics, 2018, 148, 184702.	3.0	13
64	Melting of sulfur hexafluoride clusters by molecular dynamics simulation. Molecular Physics, 1992, 76, 1079-1091.	1.7	12
65	United atom forcefield for vapor-liquid equilibrium (VLE) properties of cyclic and polycyclic compounds from Monte Carlo simulations. Fluid Phase Equilibria, 2019, 481, 28-43.	2.5	12
66	Grain boundary premelting in crystalline benzene as studied by proton N.M.R.. Journal De Physique, 1990, 51, 2489-2499.	1.8	11
67	Transport Coefficients of Xylene Isomers. Journal of Physical Chemistry B, 2002, 106, 13010-13017.	2.6	10
68	Rheological behavior of aqueous polyacrylamide solutions determined by dissipative particle dynamics and comparison to experiments. Europhysics Letters, 2012, 97, 34007.	2.0	10
69	On a variational approach to the Soret coefficient. Journal of Chemical Physics, 2006, 125, 164508.	3.0	9
70	Assessment of an anisotropic coarse-grained model for cis-1,4-polybutadiene: a bottom-up approach. Soft Matter, 2021, 17, 621-636.	2.7	9
71	Determination of average molecular weights of high-boiling aromatic oil fractions by 13C and 1H nuclear magnetic resonance. Fuel, 1989, 68, 1158-1161.	6.4	8
72	A model for the static friction behaviour of nanolubricated contacts. Thin Solid Films, 1998, 330, 21-26.	1.8	8

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73	Dynamic disorder in stable and metastable thiophene. - II. Non Lorentzian nuclear relaxation and glass transition. Journal De Physique, 1989, 50, 855-859.	1.8	7
74	Surface melting of a molecular crystal by computer simulations. Surface Science, 1993, 287-288, 866-870.	1.9	7
75	Gas Permeation in Semicrystalline Polyethylene as Studied by Molecular Simulation and Elastic Model. Oil and Gas Science and Technology, 2015, 70, 227-235.	1.4	7
76	Premelting, defects and self diffusion in molecular crystals. Solid State Communications, 1988, 67, 1017-1018.	1.9	6
77	Flux expressions and NEMD perturbations for models of semi-flexible molecules. Molecular Physics, 2001, 99, 1139-1149.	1.7	6
78	Simulations of Interfacial Tension of Liquidâ€“Liquid Ternary Mixtures Using Optimized Parametrization for Coarse-Grained Models. Journal of Chemical Theory and Computation, 2018, 14, 4438-4454.	5.3	6
79	Thermodynamically Consistent Force Field for Coarse-Grained Modeling of Aqueous Electrolyte Solution. Journal of Physical Chemistry B, 2019, 123, 2424-2431.	2.6	6
80	Dynamic disorder in stable and metastable thiophene. - I. N. M. R. lineshape study and structurally based interpretations. Journal De Physique, 1988, 49, 281-288.	1.8	6
81	Factors influencing properties of interfacial regions in semicrystalline polyethylene: A molecular dynamics simulation study. Polymer, 2013, 54, 3586-3593.	3.8	5
82	Molecular simulation of the thermodynamics, structural and transport properties of the liquid binary mixture methane+nitrogen. Journal of Molecular Liquids, 2014, 200, 298-304.	4.9	5
83	The phases and dynamics of succinonitrile : An NMR absorption line study. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1990, 87, 1821-1833.	0.2	4
84	Molecular simulation of a reverse osmosis polyamide membrane layer. In silico synthesis using different reactant concentration ratios. Journal of Membrane Science, 2022, 643, 120010.	8.2	4
85	Molecular relaxation and microstructures in glassy crystals. Journal of Physics C: Solid State Physics, 1988, 21, 731-737.	1.5	3
86	Preventing iron(ii) precipitation in aqueous systems using polyacrylic acid: some molecular insights. Physical Chemistry Chemical Physics, 2018, 20, 18056-18065.	2.8	3
87	Experimental Characterization of Commercial and Synthesized Aromatic Polyamide Films for Reverse Osmosis Membranes. Industrial & Engineering Chemistry Research, 2021, 60, 2898-2910.	3.7	2
88	Structural characterization of a crude oil by one and two dimensional nuclear magnetic resonance spectroscopy. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1992, 89, 533-539.	0.2	2
89	SCCO: Thermodiffusion for the Oil and Gas Industry. Research for Development, 2019, , 171-190.	0.4	2
90	Molecular Simulations As a Tool for Predicting Phase Equilibria and Transport Properties of Fluids. Oil & Gas Science & Technology, 1998, 53, 329-333.	0.2	0

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91	Low-Temperature Vaporâ"Liquid Equilibria from Parallelized Molecular Dynamics Simulations. Application to 1- and 2-Methylnaphthalene. Journal of Physical Chemistry B, 2006, 110, 12083-12088.	2.6	0
92	PropriÃ©tÃ©s de transport en phase liquide : une approche par simulation numÃ©rique de la dynamique molÃ©culaire. Oil & Gas Science & Technology, 1996, 51, 97-104.	0.2	0