LÃ-via B PÃ¡rtay

List of Publications by Year
in descending order

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35 papers	1,405 citations	304368 22 h-index	395343 33 g-index
35 all docs	35 docs citations	35 times ranked	1297 citing authors

#	Article	IF	Citations
1	Nested sampling for physical scientists. Nature Reviews Methods Primers, 2022, 2, .	11.8	40
2	Insight into Liquid Polymorphism from the Complex Phase Behavior of a Simple Model. Physical Review Letters, 2021, 127, 015701.	2.9	7
3	Nested sampling for materials. European Physical Journal B, 2021, 94, 1.	0.6	13
4	Machine-learned interatomic potentials for alloys and alloy phase diagrams. Npj Computational Materials, 2021, 7, .	3.5	75
5	Pressureâ€“Temperature Phase Diagram of Lithium, Predicted by Embedded Atom Model Potentials. Journal of Physical Chemistry B, 2020, 124, 6015-6023.	1.2	11
6	Thermodynamics and the potential energy landscape: case study of small water clusters. Physical Chemistry Chemical Physics, 2019, 21, 7305-7312.	1.3	9
7	On the performance of interatomic potential models of iron: Comparison of the phase diagrams. Computational Materials Science, 2018, 149, 153-157.	1.4	18
8	Direct Computation of the Quantum Partition Function by Path-Integral Nested Sampling. Journal of Chemical Theory and Computation, 2018, 14, 4353-4359.	2.3	8
9	Constant-pressure nested sampling with atomistic dynamics. Physical Review E, 2017, 96, 043311.	0.8	27
10	Polytypism in the ground state structure of the Lennard-Jonesium. Physical Chemistry Chemical Physics, 2017, 19, 19369-19376.	1.3	21
11	Determining pressure-temperature phase diagrams of materials. Physical Review B, 2016, 93, .	1.1	49
12	Nested sampling for materials: The case of hard spheres. Physical Review E, 2014, 89, 022302.	0.8	31
13	Diffusive nested sampling. Statistics and Computing, 2011, 21, 649-656.	0.8	101
14	Computer simulation and ITIM analysis of the surface of waterâ€“methanol mixtures containing traces of water. Journal of Molecular Liquids, 2010, 153, 88-93.	2.3	26
15	Molecular level properties of the free water surface and different organic liquid/water interfaces, as seen from ITIM analysis of computer simulation results. Journal of Physics Condensed Matter, 2010, 22, 284112.	0.7	40
16	Efficient Sampling of Atomic Configurational Spaces. Journal of Physical Chemistry B, 2010, 114, 10502-10512.	1.2	89
17	Temperature and Pressure Dependence of the Properties of the Liquidâ”Liquid Interface. A Computer Simulation and Identification of the Truly Interfacial Molecules Investigation of the Waterâ”Benzene System. Journal of Physical Chemistry C, 2010, 114, 21681-21693.	1.5	33
18	Structure of the Liquidâ”Vapor Interface of Waterâ”Acetonitrile Mixtures As Seen from Molecular Dynamics Simulations and Identification of Truly Interfacial Molecules Analysis. Journal of Physical Chemistry C, 2009, 113, 18173-18183.	1.5	45

#	Article	IF	Citations
19	A new method for determining the interfacial molecules and characterizing the surface roughness in computer simulations. Application to the liquidâ€“vapor interface of water. Journal of Computational Chemistry, 2008, 29, 945-956.	1.5	181
20	Behavior of molecular oxygen at the liquidâ€“liquid interface: A molecular dynamics simulation study. Chemical Physics Letters, 2008, 457, 78-81.	1.2	1
21	AÂTwo-step Aggregation Scheme of Bile Acid Salts, as Seen From Computer Simulations. , 2008, , 181-187.		4
22	Structural and thermodynamic properties of different phases of supercooled liquid water. Journal of Chemical Physics, 2008, 128, 244503.	1.2	31
23	Molecular level structure of the liquid/liquid interface. Molecular dynamics simulation and ITIM analysis of the water-CCl4 system. Physical Chemistry Chemical Physics, 2008, 10, 4754.	1.3	50
24	Counterion Binding in the Aqueous Solutions of Bile Acid Salts, as Studied by Computer Simulation Methods. Langmuir, 2008, 24, 10729-10736.	1.6	24
25	Properties of Free Surface of Waterâ^'Methanol Mixtures. Analysis of the Truly Interfacial Molecular Layer in Computer Simulation. Journal of Physical Chemistry B, 2008, 112, 5428-5438.	1.2	69
26	Structure of coexisting liquid phases of supercooled water: Analogy with ice polymorphs. Journal of Chemical Physics, 2007, 126, 241103.	1.2	10
27	Molecular Aggregates in Aqueous Solutions of Bile Acid Salts. Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2007, 111, 9886-9896.	1.2	132
28	Free-Energy Profile of Small Solute Molecules at the Free Surfaces of Water and Ice, as Determined by Cavity Insertion Widom Calculations. Journal of Physical Chemistry C, 2007, 111, 9407-9416.	1.5	45
29	Adsorption of Octyl Cyanide at the Free Water Surface as Studied by Monte Carlo Simulation. Journal of Physical Chemistry B, 2007, 111, 5885-5895.	1.2	5
30	Percolation Transition in Supercritical Water: A Monte Carlo Simulation Study. Journal of Physical Chemistry B, 2007, 111, 7603-7609.	1.2	36
31	Formation of mesoscopic water networks in aqueous systems. Physical Chemistry Chemical Physics, 2007, 9, 1341-1346.	1.3	37
32	Morphology of Bile Salt Micelles as Studied by Computer Simulation Methods. Langmuir, 2007, 23, 12322-12328.	1.6	84
33	Counterion and Surface Density Dependence of the Adsorption Layer of Ionic Surfactants at the Vaporâ^'Aqueous Solution Interface:Â A Computer Simulation Study. Journal of Physical Chemistry B, 2007, 111, 1769-1774.	1.2	43
34	Investigation of the saturated adsorption layer of 5-cyano-biphenyl and 5-cyano-terphenyl at the free water surface by Monte Carlo simulation. Journal of Molecular Liquids, 2007, 136, 249-256.	2.3	9
35	Stability of the high-density Jagla liquid in 2D: sensitivity to parameterisation. Soft Matter, 0, , .	1.2	1