

# 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	A new method for determining the interfacial molecules and characterizing the surface roughness in computer simulations. Application to the liquid-vapor interface of water. <i>Journal of Computational Chemistry</i> , 2008, 29, 945-956.	1.5	181
2	Molecular Aggregates in Aqueous Solutions of Bile Acid Salts. <i>Molecular Dynamics Simulation Study. Journal of Physical Chemistry B</i> , 2007, 111, 9886-9896.	1.2	132
3	Diffusive nested sampling. <i>Statistics and Computing</i> , 2011, 21, 649-656.	0.8	101
4	Efficient Sampling of Atomic Configurational Spaces. <i>Journal of Physical Chemistry B</i> , 2010, 114, 10502-10512.	1.2	89
5	Morphology of Bile Salt Micelles as Studied by Computer Simulation Methods. <i>Langmuir</i> , 2007, 23, 12322-12328.	1.6	84
6	Machine-learned interatomic potentials for alloys and alloy phase diagrams. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	75
7	Properties of Free Surface of Water-Methanol Mixtures. Analysis of the Truly Interfacial Molecular Layer in Computer Simulation. <i>Journal of Physical Chemistry B</i> , 2008, 112, 5428-5438.	1.2	69
8	Molecular level structure of the liquid/liquid interface. Molecular dynamics simulation and ITIM analysis of the water-CCl <sub>4</sub> system. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 4754.	1.3	50
9	Determining pressure-temperature phase diagrams of materials. <i>Physical Review B</i> , 2016, 93, .	1.1	49
10	Free-Energy Profile of Small Solute Molecules at the Free Surfaces of Water and Ice, as Determined by Cavity Insertion Widom Calculations. <i>Journal of Physical Chemistry C</i> , 2007, 111, 9407-9416.	1.5	45
11	Structure of the Liquid-Vapor Interface of Water-Acetonitrile Mixtures As Seen from Molecular Dynamics Simulations and Identification of Truly Interfacial Molecules Analysis. <i>Journal of Physical Chemistry C</i> , 2009, 113, 18173-18183.	1.5	45
12	Counterion and Surface Density Dependence of the Adsorption Layer of Ionic Surfactants at the Vapor-Aqueous Solution Interface: A Computer Simulation Study. <i>Journal of Physical Chemistry B</i> , 2007, 111, 1769-1774.	1.2	43
13	Molecular level properties of the free water surface and different organic liquid/water interfaces, as seen from ITIM analysis of computer simulation results. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 284112.	0.7	40
14	Nested sampling for physical scientists. <i>Nature Reviews Methods Primers</i> , 2022, 2, .	11.8	40
15	Formation of mesoscopic water networks in aqueous systems. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 1341-1346.	1.3	37
16	Percolation Transition in Supercritical Water: A Monte Carlo Simulation Study. <i>Journal of Physical Chemistry B</i> , 2007, 111, 7603-7609.	1.2	36
17	Temperature and Pressure Dependence of the Properties of the Liquid-Liquid Interface. A Computer Simulation and Identification of the Truly Interfacial Molecules Investigation of the Water-Benzene System. <i>Journal of Physical Chemistry C</i> , 2010, 114, 21681-21693.	1.5	33
18	Structural and thermodynamic properties of different phases of supercooled liquid water. <i>Journal of Chemical Physics</i> , 2008, 128, 244503.	1.2	31

#	ARTICLE	IF	CITATIONS
19	Nested sampling for materials: The case of hard spheres. <i>Physical Review E</i> , 2014, 89, 022302.	0.8	31
20	Constant-pressure nested sampling with atomistic dynamics. <i>Physical Review E</i> , 2017, 96, 043311.	0.8	27
21	Computer simulation and ITIM analysis of the surface of water-methanol mixtures containing traces of water. <i>Journal of Molecular Liquids</i> , 2010, 153, 88-93.	2.3	26
22	Counterion Binding in the Aqueous Solutions of Bile Acid Salts, as Studied by Computer Simulation Methods. <i>Langmuir</i> , 2008, 24, 10729-10736.	1.6	24
23	Polytypism in the ground state structure of the Lennard-Jonesium. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 19369-19376.	1.3	21
24	On the performance of interatomic potential models of iron: Comparison of the phase diagrams. <i>Computational Materials Science</i> , 2018, 149, 153-157.	1.4	18
25	Nested sampling for materials. <i>European Physical Journal B</i> , 2021, 94, 1.	0.6	13
26	Pressure-Temperature Phase Diagram of Lithium, Predicted by Embedded Atom Model Potentials. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6015-6023.	1.2	11
27	Structure of coexisting liquid phases of supercooled water: Analogy with ice polymorphs. <i>Journal of Chemical Physics</i> , 2007, 126, 241103.	1.2	10
28	Investigation of the saturated adsorption layer of 5-cyano-biphenyl and 5-cyano-terphenyl at the free water surface by Monte Carlo simulation. <i>Journal of Molecular Liquids</i> , 2007, 136, 249-256.	2.3	9
29	Thermodynamics and the potential energy landscape: case study of small water clusters. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7305-7312.	1.3	9
30	Direct Computation of the Quantum Partition Function by Path-Integral Nested Sampling. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4353-4359.	2.3	8
31	Insight into Liquid Polymorphism from the Complex Phase Behavior of a Simple Model. <i>Physical Review Letters</i> , 2021, 127, 015701.	2.9	7
32	Adsorption of Octyl Cyanide at the Free Water Surface as Studied by Monte Carlo Simulation. <i>Journal of Physical Chemistry B</i> , 2007, 111, 5885-5895.	1.2	5
33	Two-step Aggregation Scheme of Bile Acid Salts, as Seen From Computer Simulations. , 2008, , 181-187.		4
34	Behavior of molecular oxygen at the liquid-liquid interface: A molecular dynamics simulation study. <i>Chemical Physics Letters</i> , 2008, 457, 78-81.	1.2	1
35	Stability of the high-density Jagla liquid in 2D: sensitivity to parameterisation. <i>Soft Matter</i> , 0, , .	1.2	1