Simon Stephan

List of Publications by Year
in descending order

29	971	394421 19	477307 29
papers	citations	h-index	g-index

31	31	31	414
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Thermophysical Properties of the Lennard-Jones Fluid: Database and Data Assessment. Journal of Chemical Information and Modeling, 2019, 59, 4248-4265.	5.4	101
2	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" id="mml56" display="inline" overflow="scroll" altimg="si19.gif"><mml:mi>m</mml:mi><mml:mi>s</mml:mi><mml:mn>2</mml:mn></mml:math>: A molecular simulation tool for thermodynamic properties, release 3.0. Computer Physics Communications, 2017, 221, 343-351.	7.5	70
3	MolMod â€“ an open access database of force fields for molecular simulations of fluids. Molecular Simulation, 2019, 45, 806-814.	2.0	65
4	Equation of state for the Lennard-Jones truncated and shifted fluid with a cut-off radius of 2.5â€‰ïƒ based on perturbation theory and its applications to interfacial thermodynamics. Molecular Physics, 2018, 116, 2083-2094.	1.7	61
5	Vaporâ^'Liquid Interface of the Lennard-Jones Truncated and Shifted Fluid: Comparison of Molecular Simulation, Density Gradient Theory, and Density Functional Theory. Journal of Physical Chemistry C, 2018, 122, 24705-24715.	3.1	61
6	Review and comparison of equations of state for the Lennard-Jones fluid. Fluid Phase Equilibria, 2020, 523, 112772.	2.5	58
7	Enrichment at vapourâ€“liquid interfaces of mixtures: establishing a link between nanoscopic and macroscopic properties. International Reviews in Physical Chemistry, 2020, 39, 319-349.	2.3	56
8	Interfacial properties of binary Lennard-Jones mixtures by molecular simulation and density gradient theory. Journal of Chemical Physics, 2019, 150, 174704.	3.0	53
9	Round Robin Study: Molecular Simulation of Thermodynamic Properties from Models with Internal Degrees of Freedom. Journal of Chemical Theory and Computation, 2017, 13, 4270-4280.	5.3	48
10	Influence of dispersive long-range interactions on properties of vapourâ€“liquid equilibria and interfaces of binary Lennard-Jones mixtures. Molecular Physics, 2020, 118, e1699185.	1.7	36
11	Molecular interactions at vapor-liquid interfaces: Binary mixtures of simple fluids. Physical Review E, 2020, 101, 012802.	2.1	36
12	Mass transfer through vapourâ€“liquid interfaces: a molecular dynamics simulation study. Molecular Physics, 2021, 119, e1810798.	1.7	36
13	Interfacial properties of binary mixtures of simple fluids and their relation to the phase diagram. Physical Chemistry Chemical Physics, 2020, 22, 12544-12564.	2.8	35
14	ms2: A molecular simulation tool for thermodynamic properties, release 4.0. Computer Physics Communications, 2021, 262, 107860.	7.5	31
15	The Influence of Lubrication and the Solidâ€“Fluid Interaction on Thermodynamic Properties in a Nanoscopic Scratching Process. Langmuir, 2019, 35, 16948-16960.	3.5	29
16	Vapor-liquid interfacial properties of the system cyclohexaneÂ+ CO2: Experiments, molecular simulation and density gradient theory. Fluid Phase Equilibria, 2020, 518, 112583.	2.5	29
17	Molecular dynamics and phase field simulations of droplets on surfaces with wettability gradient. Computer Methods in Applied Mechanics and Engineering, 2020, 361, 112773.	6.6	27
18	Molecular Dynamics Simulation Study of Mechanical Effects of Lubrication on a Nanoscale Contact Process. Tribology Letters, 2018, 66, 1.	2.6	25

#	Article	IF	Citations
19	Characteristic Curves of the Lennard-Jones Fluid. International Journal of Thermophysics, 2020, 41, 147.	2.1	20
20	Molecular Dynamics Study of Wetting and Adsorption of Binary Mixtures of the Lennard-Jones Truncated and Shifted Fluid on a Planar Wall. Langmuir, 2021, 37, 7405-7419.	3.5	19
21	Effects of Lubrication on the Friction in Nanometric Machining Processes: A Molecular Dynamics Approach. Applied Mechanics and Materials, 0, 869, 85-93.	0.2	15
22	Molecular dynamics simulation study of heat transfer across solidâ€“fluid interfaces in a simple model system. Molecular Physics, 2022, 120, .	1.7	13
23	A Force Field for Poly(oxymethylene) Dimethyl Ethers (OMEn). Journal of Chemical Theory and Computation, 2020, 16, 2517-2528.	5.3	12
24	Effects of Lubrication on Friction and Heat Transfer in Machining Processes on the Nanoscale: A Molecular Dynamics Approach. Procedia CIRP, 2018, 67, 296-301.	1.9	11
25	SkaSim â€“ Scalable HPC Software for Molecular Simulation in the Chemical Industry. Chemie-Ingenieur-Technik, 2018, 90, 295-306.	0.8	7
26	Assessment of thermodynamic models via Jouleâ€“Thomson inversion. Fluid Phase Equilibria, 2022, 556, 113401.	2.5	7
27	Reproducibility of atomistic friction computer experiments: a molecular dynamics simulation study. Molecular Simulation, 2021, 47, 1509-1521.	2.0	6
28	Sensorkonzept zur Bestimmung der Dampffeuchte und des thermischen Zustandspunkts von Nassdampf mittels Schwingungsspektroskopie. TM Technisches Messen, 2017, 84, 719-733.	0.7	1
29	Phase Field Modeling of Dynamic Surface Wetting informed by Molecular Simulations. Proceedings in Applied Mathematics and Mechanics, 2021, 21, .	0.2	1