

Paul J Van Maaren

List of Publications by Year in descending order

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17
papers

2,938
citations

567281

15
h-index

888059

17
g-index

17
all docs

17
docs citations

17
times ranked

3755
citing authors

#	ARTICLE	IF	CITATIONS
1	Force Field Benchmark of Organic Liquids: Density, Enthalpy of Vaporization, Heat Capacities, Surface Tension, Isothermal Compressibility, Volumetric Expansion Coefficient, and Dielectric Constant. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 61-74.	5.3	609
2	A systematic study of water models for molecular simulation: Derivation of water models optimized for use with a reaction field. <i>Journal of Chemical Physics</i> , 1998, 108, 10220-10230.	3.0	581
3	Thermodynamics of Hydrogen Bonding in Hydrophilic and Hydrophobic Media. <i>Journal of Physical Chemistry B</i> , 2006, 110, 4393-4398.	2.6	404
4	Dynamic properties of water/alcohol mixtures studied by computer simulation. <i>Journal of Chemical Physics</i> , 2003, 119, 7308-7317.	3.0	255
5	The Origin of Layer Structure Artifacts in Simulations of Liquid Water. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1-11.	5.3	195
6	Atomistic simulation of ion solvation in water explains surface preference of halides. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 6838-6842.	7.1	192
7	Molecular Dynamics Simulations of Water with Novel Shell-Model Potentials. <i>Journal of Physical Chemistry B</i> , 2001, 105, 2618-2626.	2.6	162
8	GROMACS molecule & liquid database. <i>Bioinformatics</i> , 2012, 28, 752-753.	4.1	161
9	Properties of Organic Liquids when Simulated with Long-Range Lennard-Jones Interactions. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2938-2944.	5.3	116
10	Large-scale calculations of gas phase thermochemistry: Enthalpy of formation, standard entropy, and heat capacity. <i>Journal of Chemical Physics</i> , 2016, 145, .	3.0	60
11	Thermodynamics of hydronium and hydroxide surface solvation. <i>Chemical Science</i> , 2014, 5, 1745.	7.4	56
12	The Alexandria library, a quantum-chemical database of molecular properties for force field development. <i>Scientific Data</i> , 2018, 5, 180062.	5.3	45
13	Phase-Transferable Force Field for Alkali Halides. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5933-5948.	5.3	35
14	Towards phase transferable potential functions: Methodology and application to nitrogen. <i>Journal of Chemical Physics</i> , 1995, 103, 2272-2285.	3.0	33
15	Polarizable Drude Model with $\langle i \rangle s \langle /i \rangle$ -Type Gaussian or Slater Charge Density for General Molecular Mechanics Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5553-5566.	5.3	27
16	A potential for molecular simulation of compounds with linear moieties. <i>Journal of Chemical Physics</i> , 2020, 153, 084503.	3.0	5
17	2D Monte Carlo simulations of radiation effects on non-equilibrium colloid growth. <i>Journal of Physics Condensed Matter</i> , 1994, 6, 9053-9064.	1.8	2