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