Esther Heid

List of Publications by Citations

26	292	11	16
papers	citations	h-index	g-index
40	409	4.5	3.98
ext. papers	ext. citations	avg, IF	L-index

#	Paper	IF	Citations
26	Quantum mechanical determination of atomic polarizabilities of ionic liquids. *Physical Chemistry Chemical Physics*, **2018**, 20, 10992-10996	3.6	30
25	Additive polarizabilities in ionic liquids. *Physical Chemistry Chemical Physics*, **2016**, 18, 1665-70	3.6	27
24	Thioglycolate-based task-specific ionic liquids: Metal extraction abilities vs acute algal toxicity. *Journal of Hazardous Materials*, **2017**, 340, 113-119	12.8	23
23	Regio-selectivity prediction with a machine-learned reaction representation and on-the-fly quantum mechanical descriptors. *Chemical Science*, **2020**, 12, 2198-2208	9.4	21
22	Solvation dynamics in polar solvents and imidazolium ionic liquids: failure of linear response approximations. *Physical Chemistry Chemical Physics*, **2018**, 20, 5246-5255	3.6	20
21	Evaluating excited state atomic polarizabilities of chromophores. *Physical Chemistry Chemical Physics*, **2018**, 20, 8554-8563	3.6	17
20	On the validity of linear response approximations regarding the solvation dynamics of polyatomic solutes. *Physical Chemistry Chemical Physics*, **2017**, 19, 10940-10950	3.6	15
19	The small impact of various partial charge distributions in ground and excited state on the computational Stokes shift of 1-methyl-6-oxyquinolinium betaine in diverse water models. *Journal of Chemical Physics*, **2016**, 145, 164506	3.9	15
18	Langevin behavior of the dielectric decrement in ionic liquid water mixtures. *Physical Chemistry Chemical Physics*, **2018**, 20, 15106-15117	3.6	13
17	Understanding the Nature of Nuclear Magnetic Resonance Relaxation by Means of Fast-Field-Cycling Relaxometry and Molecular Dynamics Simulations-The Validity of Relaxation Models. *Journal of Physical Chemistry Letters*, **2020**, 11, 2165-2170	6.4	12
16	Additive polarizabilities of halides in ionic liquids and organic solvents. *Journal of Chemical Physics*, **2018**, 149, 044302	3.9	11
15	Effect of a Tertiary Butyl Group on Polar Solvation Dynamics in Aqueous Solution: A Computational Approach. *Journal of Physical Chemistry B*, **2017**, 121, 9639-9646	3.4	10
14	Toward Prediction of Electrostatic Parameters for Force Fields That Explicitly Treat Electronic Polarization. *Journal of Chemical Theory and Computation*, **2019**, 15, 2460-2469	6.4	10
13	Computational solvation dynamics of oxyquinolinium betaine linked to trehalose. *Journal of Chemical Physics*, **2016**, 145, 164507	3.9	10
12	Solvation dynamics: improved reproduction of the time-dependent Stokes shift with polarizable empirical force field chromophore models. *Physical Chemistry Chemical Physics*, **2019**, 21, 17703-17710	3.6	9
11	Fundamental limitations of the time-dependent Stokes shift for investigating protein hydration dynamics. *Physical Chemistry Chemical Physics*, **2019**, 21, 4435-4443	3.6	7
10	Polarizability in ionic liquid simulations causes hidden breakdown of linear response theory. *Physical Chemistry Chemical Physics*, **2019**, 21, 1023-1028	3.6	7

9	Polarizable molecular dynamics simulations of ionic liquids: Influence of temperature control. *Journal of Chemical Physics*, **2020**, 152, 094105	3.9	7
8	The physical significance of the Kamlet-Taft * parameter of ionic liquids. *Physical Chemistry Chemical Physics*, **2021**, 23, 1616-1626	3.6	7
7	Computational spectroscopy of trehalose, sucrose, maltose, and glucose: A comprehensive study of TDSS, NQR, NOE, and DRS. *Journal of Chemical Physics*, **2019**, 150, 175102	3.9	5
6	Changes in protein hydration dynamics by encapsulation or crowding of ubiquitin: strong correlation between time-dependent Stokes shift and intermolecular nuclear Overhauser effect.. *RSC Advances*, **2019**, 9, 36982-36993	3.7	4
5	Solvation of anthraquinone and TEMPO redox-active species in acetonitrile using a polarizable force field. *Journal of Chemical Physics*, **2021**, 155, 074504	3.9	4
4	Polarizable General Force Field for Drug-Like Molecules: Drude General Force Field (DGenFF). *Biophysical Journal*, **2019**, 116, 142a	2.9	2
3	Computational solvation dynamics: Implementation, application, and validation. *Annual Reports in Computational Chemistry*, **2020**, 93-154	1.8	1
2	Dielectric spectroscopy and time dependent Stokes shift: two faces of the same coin?. *Physical Chemistry Chemical Physics*, **2020**, 22, 18388-18399	3.6	1
1	EHreact: Extended Hasse Diagrams for the Extraction and Scoring of Enzymatic Reaction Templates. *Journal of Chemical Information and Modeling*, **2021**, 61, 4949-4961	6.1	1