

Esther Heid

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

26

papers

292

citations

11

h-index

16

g-index

40

ext. papers

409

ext. citations

4.5

avg, IF

3.98

L-index

#	Paper	IF	Citations
26	The physical significance of the Kamlet-Taft * parameter of ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 1616-1626	3.6	7
25	Solvation of anthraquinone and TEMPO redox-active species in acetonitrile using a polarizable force field. <i>Journal of Chemical Physics</i> , 2021 , 155, 074504	3.9	4
24	EHreact: Extended Hasse Diagrams for the Extraction and Scoring of Enzymatic Reaction Templates. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 4949-4961	6.1	1
23	Polarizable molecular dynamics simulations of ionic liquids: Influence of temperature control. <i>Journal of Chemical Physics</i> , 2020 , 152, 094105	3.9	7
22	Understanding the Nature of Nuclear Magnetic Resonance Relaxation by Means of Fast-Field-Cycling Relaxometry and Molecular Dynamics Simulations-The Validity of Relaxation Models. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 2165-2170	6.4	12
21	Computational solvation dynamics: Implementation, application, and validation. <i>Annual Reports in Computational Chemistry</i> , 2020 , 93-154	1.8	1
20	Dielectric spectroscopy and time dependent Stokes shift: two faces of the same coin?. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 18388-18399	3.6	1
19	Regio-selectivity prediction with a machine-learned reaction representation and on-the-fly quantum mechanical descriptors. <i>Chemical Science</i> , 2020 , 12, 2198-2208	9.4	21
18	Fundamental limitations of the time-dependent Stokes shift for investigating protein hydration dynamics. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 4435-4443	3.6	7
17	Polarizability in ionic liquid simulations causes hidden breakdown of linear response theory. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 1023-1028	3.6	7
16	Computational spectroscopy of trehalose, sucrose, maltose, and glucose: A comprehensive study of TDSS, NQR, NOE, and DRS. <i>Journal of Chemical Physics</i> , 2019 , 150, 175102	3.9	5
15	Toward Prediction of Electrostatic Parameters for Force Fields That Explicitly Treat Electronic Polarization. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 2460-2469	6.4	10
14	Solvation dynamics: improved reproduction of the time-dependent Stokes shift with polarizable empirical force field chromophore models. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 17703-17710	3.6	9
13	Polarizable General Force Field for Drug-Like Molecules: Drude General Force Field (DGenFF). <i>Biophysical Journal</i> , 2019 , 116, 142a	2.9	2
12	Changes in protein hydration dynamics by encapsulation or crowding of ubiquitin: strong correlation between time-dependent Stokes shift and intermolecular nuclear Overhauser effect.. <i>RSC Advances</i> , 2019 , 9, 36982-36993	3.7	4
11	Evaluating excited state atomic polarizabilities of chromophores. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 8554-8563	3.6	17
10	Quantum mechanical determination of atomic polarizabilities of ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 10992-10996	3.6	30

9	Solvation dynamics in polar solvents and imidazolium ionic liquids: failure of linear response approximations. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 5246-5255	3.6	20
8	Additive polarizabilities of halides in ionic liquids and organic solvents. <i>Journal of Chemical Physics</i> , 2018 , 149, 044302	3.9	11
7	Langevin behavior of the dielectric decrement in ionic liquid water mixtures. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 15106-15117	3.6	13
6	Effect of a Tertiary Butyl Group on Polar Solvation Dynamics in Aqueous Solution: A Computational Approach. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 9639-9646	3.4	10
5	Thioglycolate-based task-specific ionic liquids: Metal extraction abilities vs acute algal toxicity. <i>Journal of Hazardous Materials</i> , 2017 , 340, 113-119	12.8	23
4	On the validity of linear response approximations regarding the solvation dynamics of polyatomic solutes. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 10940-10950	3.6	15
3	Additive polarizabilities in ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 1665-70	3.6	27
2	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. <i>Journal of Chemical Physics</i> , 2016 , 145, 164506	3.9	15
1	Computational solvation dynamics of oxyquinolinium betaine linked to trehalose. <i>Journal of Chemical Physics</i> , 2016 , 145, 164507	3.9	10