Christian Schrder

List of Publications by Year in Descending Order

88 papers	2,715 citations	30 h-index	49 g-index
93 ext. papers	3,112 ext. citations	4.8 avg, IF	5.81 L-index

#	Paper	IF	Citations
88	The influence of the cation structure on the basicity-related polarity of ionic liquids. *Physical Chemistry Chemical Physics*, **2021**, 23, 26750-26760	3.6	1
87	Charge delocalization and hyperpolarizability in ionic liquids. *Journal of Molecular Liquids*, **2021**, 118153	6	0
86	Surface-active ionic liquids: A review. *Journal of Molecular Liquids*, **2021**, 347, 118160	6	7
85	Non-additive electronic polarizabilities of ionic liquids: Charge delocalization effects. *Journal of Molecular Liquids*, **2021**, 346, 117099	6	2
84	The physical significance of the Kamlet-Taft * parameter of ionic liquids. *Physical Chemistry Chemical Physics*, **2021**, 23, 1616-1626	3.6	7
83	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
82	Comparison between ab initio and polarizable molecular dynamics simulations of 1-butyl-3-methylimidazolium tetrafluoroborate and chloride in water. *Journal of Molecular Liquids*, **2021**, 337, 116521	6	2
81	The Intermolecular NOE Depends on Isotope Selection: Short Range vs Long Range Behavior. *Journal of Physical Chemistry Letters*, **2021**, 12, 8658-8663	6.4	1
80	Polarizable molecular dynamics simulations of ionic liquids: Influence of temperature control. *Journal of Chemical Physics*, **2020**, 152, 094105	3.9	7
79	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
78	Computational solvation dynamics: Implementation, application, and validation. *Annual Reports in Computational Chemistry*, **2020**, 93-154	1.8	1
77	Polarizable MD simulations of ionic liquids: How does additional charge transfer change the dynamics?. *Physical Chemistry Chemical Physics*, **2020**, 22, 467-477	3.6	10
76	Enantiomerization of Axially Chiral Biphenyls: Polarizable MD Simulations in Water and Butylmethylether. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	1
75	Dielectric spectroscopy and time dependent Stokes shift: two faces of the same coin?. *Physical Chemistry Chemical Physics*, **2020**, 22, 18388-18399	3.6	1
74	Polarizability in ionic liquid simulations causes hidden breakdown of linear response theory. *Physical Chemistry Chemical Physics*, **2019**, 21, 1023-1028	3.6	7
73	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. *Chemical Reviews*, **2019**, 119, 7940-7995	68.1	206
72	Computational analysis of conductivity contributions in an ionic liquid mixture of 1-ethyl-3-methylimidazolium dicyanamide and tetrafluoroborate. *Journal of Molecular Liquids*, **2019**, 288, 110993	6	3

71	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
70	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
69	Surface-Active Ionic Liquids in Catalytic Water Splitting. *Australian Journal of Chemistry*, **2019**, 72, 34	1.2	7
68	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
67	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
66	Ion-Tagged Chiral Ligands for Asymmetric Transfer Hydrogenations in Aqueous Medium. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 3414-3423	8.3	10
65	Evaluating excited state atomic polarizabilities of chromophores. *Physical Chemistry Chemical Physics*, **2018**, 20, 8554-8563	3.6	17
64	Quantum mechanical determination of atomic polarizabilities of ionic liquids. *Physical Chemistry Chemical Physics*, **2018**, 20, 10992-10996	3.6	30
63	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
62	Computational solvation analysis of biomolecules in aqueous ionic liquid mixtures : From large flexible proteins to small rigid drugs. *Biophysical Reviews*, **2018**, 10, 825-840	3.7	10
61	Additive polarizabilities of halides in ionic liquids and organic solvents. *Journal of Chemical Physics*, **2018**, 149, 044302	3.9	11
60	Selective Hydrogenation of Aldehydes Using a Well-Defined Fe(II) PNP Pincer Complex in Biphasic Medium. *ChemCatChem*, **2018**, 10, 4386-4394	5.2	7
59	Molecular dynamics simulation of aqueous 1-dodecyl-3-methylimidazolium chloride: Emerging micelles. *Journal of Molecular Liquids*, **2018**, 272, 766-777	6	7
58	A shell-resolved analysis of preferential solvation of coffee ingredients in aqueous mixtures of the ionic liquid 1-ethyl-3-methylimidazolium acetate. *Journal of Chemical Physics*, **2018**, 148, 193819	3.9	13
57	Langevin behavior of the dielectric decrement in ionic liquid water mixtures. *Physical Chemistry Chemical Physics*, **2018**, 20, 15106-15117	3.6	13
56	Computational analysis of the solvation of coffee ingredients in aqueous ionic liquid mixtures. *RSC Advances*, **2017**, 7, 3495-3504	3.7	15
55	Proteins in Ionic Liquids: Current Status of Experiments and Simulations. *Topics in Current Chemistry* , **2017**, 375, 25	7.2	86
54	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

53	Thioglycolate-based task-specific ionic liquids: Metal extraction abilities vs acute algal toxicity. *Journal of Hazardous Materials*, **2017**, 340, 113-119	12.8	23
52	Proteins in Ionic Liquids: Current Status of Experiments and Simulations. *Topics in Current Chemistry Collections*, **2017**, 127-152	1.8	9
51	Proteins in Ionic Liquids: Current Status of Experiments and Simulations **2017**, 375, 1		1
50	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
49	Charged, dipolar soft matter systems from a combined microscopic-mesoscopic viewpoint. *Journal of Physics Condensed Matter*, **2016**, 28, 344008	1.8	2
48	General review of ionic liquids and their properties **2016**, 1-23		1
47	Additive polarizabilities in ionic liquids. *Physical Chemistry Chemical Physics*, **2016**, 18, 1665-70	3.6	27
46	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
45	Computational solvation dynamics of oxyquinolinium betaine linked to trehalose. *Journal of Chemical Physics*, **2016**, 145, 164507	3.9	10
44	Molecular dynamics analysis of the effect of electronic polarization on the structure and single-particle dynamics of mixtures of ionic liquids and lithium salts. *Journal of Chemical Physics*, **2016**, 145, 204507	3.9	22
43	Surface-active ionic liquids in micellar catalysis: impact of anion selection on reaction rates in nucleophilic substitutions. *Physical Chemistry Chemical Physics*, **2016**, 18, 13375-84	3.6	59
42	Orientational alignment of amyloidogenic proteins in pre-aggregated solutions. *Physical Review Letters*, **2015**, 114, 128101	7.4	10
41	Amino alcohol-derived chiral ionic liquids: structural investigations toward chiral recognition. *Tetrahedron: Asymmetry*, **2015**, 26, 1069-1082		14
40	Intrinsic Structure of the Interface of Partially Miscible Fluids: An Application to Ionic Liquids. *Journal of Physical Chemistry C*, **2015**, 119, 28448-28461	3.8	13
39	Dielectric and terahertz spectroscopy of polarizable and nonpolarizable water models: a comparative study. *Journal of Physical Chemistry A*, **2015**, 119, 1539-47	2.8	40
38	Comparing induced point-dipoles and Drude oscillators. *Physical Chemistry Chemical Physics*, **2015**, 17, 14297-306	3.6	27
37	Dielectric spectra of ionic liquids and their conversion to solvation dynamics: a detailed computational analysis of polarizable systems. *Physical Chemistry Chemical Physics*, **2014**, 16, 10999-1009	3.6	18
36	Pair dynamics and the intermolecular nuclear Overhauser effect (NOE) in liquids analysed by simulation and model theories: application to an ionic liquid. *Journal of Chemical Physics*, **2014**, 140, 184503	3.9	28

35	On the collective network of ionic liquid/water mixtures. IV. Kinetic and rotational depolarization. *Journal of Chemical Physics*, **2014**, 140, 204505	3.9	11
34	Communication: Solvation and dielectric response in ionic liquids--conductivity extension of the continuum model. *Journal of Chemical Physics*, **2013**, 138, 111102	3.9	22
33	Basic chiral ionic liquids: A novel strategy for acid-free organocatalysis. *Catalysis Today*, **2013**, 200, 80-86	5.3	26
32	Polarisabilities of alkylimidazolium ionic liquids. *Physical Chemistry Chemical Physics*, **2013**, 15, 2703-11	3.6	57
31	Exploring ionic liquid–biomass interactions: towards the improved isolation of shikimic acid from star anise pods. *RSC Advances*, **2013**, 3, 26010	3.7	41
30	Polarization effects on the solvation dynamics of coumarin C153 in ionic liquids: components and their cross-correlations. *Journal of Chemical Physics*, **2013**, 138, 204504	3.9	27
29	The effect of Thole functions on the simulation of ionic liquids with point induced dipoles at various densities. *Journal of Chemical Physics*, **2013**, 138, 204119	3.9	12
28	Micellar catalysis in aqueous-ionic liquid systems. *Chemical Communications*, **2012**, 48, 5013-5	5.8	69
27	Hydrated Ionic Liquids with and without Solute: The Influence of Water Content and Protein Solutes. *Journal of Chemical Theory and Computation*, **2012**, 8, 3911-28	6.4	43
26	Computational studies of ionic liquids: size does matter and time too. *Journal of Chemical Physics*, **2012**, 137, 094501	3.9	58
25	Comparing reduced partial charge models with polarizable simulations of ionic liquids. *Physical Chemistry Chemical Physics*, **2012**, 14, 3089-102	3.6	198
24	The influence of polarizability on the dielectric spectrum of the ionic liquid 1-ethyl-3-methylimidazolium triflate. *Physical Chemistry Chemical Physics*, **2011**, 13, 12240-8	3.6	39
23	Solvation studies of a zinc finger protein in hydrated ionic liquids. *Physical Chemistry Chemical Physics*, **2011**, 13, 6955-69	3.6	43
22	Collective translational motions and cage relaxations in molecular ionic liquids. *Journal of Chemical Physics*, **2011**, 135, 024502	3.9	51
21	Simulating polarizable molecular ionic liquids with Drude oscillators. *Journal of Chemical Physics*, **2010**, 133, 154511	3.9	77
20	Using fit functions in computational dielectric spectroscopy. *Journal of Chemical Physics*, **2010**, 132, 244109	3.9	45
19	Computational Dielectric Spectroscopy of Charged, Dipolar Systems **2010**, 279-321		4
18	Relaxation of Voronoi shells in hydrated molecular ionic liquids. *Journal of Chemical Physics*, **2009**, 131, 174509	3.9	33

17	On the collective network of ionic liquid/water mixtures. III. Structural analysis of ionic liquids on the basis of Voronoi decomposition. *Journal of Chemical Physics*, **2009**, 130, 194503	3.9	46
16	On the dielectric conductivity of molecular ionic liquids. *Journal of Chemical Physics*, **2009**, 131, 114504	3.9	53
15	Molecular dynamics simulation of heat conduction through a molecular chain. *Journal of Physical Chemistry A*, **2009**, 113, 14039-51	2.8	22
14	On the computation and contribution of conductivity in molecular ionic liquids. *Journal of Chemical Physics*, **2008**, 128, 134501	3.9	100
13	The influence of electrostatic forces on the structure and dynamics of molecular ionic liquids. *Journal of Chemical Physics*, **2008**, 128, 224503	3.9	48
12	On the collective network of ionic liquid/water mixtures. II. Decomposition and interpretation of dielectric spectra. *Journal of Chemical Physics*, **2008**, 129, 184501	3.9	83
11	Grid Services for Parallel Molecular Dynamics with NAMD and CHARMM. *Lecture Notes in Computer Science*, **2008**, 1036-1051	0.9	0
10	Impact of anisotropy on the structure and dynamics of ionic liquids: a computational study of 1-butyl-3-methyl-imidazolium trifluoroacetate. *Journal of Chemical Physics*, **2007**, 127, 044505	3.9	47
9	On the collective network of ionic liquid/water mixtures. I. Orientational structure. *Journal of Chemical Physics*, **2007**, 127, 234503	3.9	114
8	Collective rotational dynamics in ionic liquids: a computational and experimental study of 1-butyl-3-methyl-imidazolium tetrafluoroborate. *Journal of Chemical Physics*, **2007**, 126, 084511	3.9	87
7	Simulation studies of the protein-water interface. II. Properties at the mesoscopic resolution. *Journal of Chemical Physics*, **2006**, 124, 234908	3.9	36
6	Simulation studies of the protein-water interface. I. Properties at the molecular resolution. *Journal of Chemical Physics*, **2006**, 124, 234907	3.9	66
5	Simulation studies of ionic liquids: orientational correlations and static dielectric properties. *Journal of Chemical Physics*, **2006**, 125, 244506	3.9	91
4	Alchemical free energy calculations and multiple conformational substates. *Journal of Chemical Physics*, **2005**, 122, 84109	3.9	51
3	Intramolecular vibrational energy redistribution in bridged azulene-anthracene compounds: ballistic energy transport through molecular chains. *Journal of Chemical Physics*, **2004**, 121, 1754-64	3.9	84
2	Intramolecular vibrational redistribution and energy relaxation in solution: A molecular dynamics approach. *Physical Chemistry Chemical Physics*, **2002**, 4, 271-278	3.6	32
1	Quantum Yields for the Photodissociation of Iodine in Compressed Liquids and Supercritical Fluids. *Zeitschrift Fur Physikalische Chemie*, **2001**, 215,	3.1	3