

Christian Schrder

List of Publications by Citations

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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.

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	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. <i>Chemical Reviews</i> , 2019 , 119, 7940-7995	68.1	206
87	Comparing reduced partial charge models with polarizable simulations of ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 3089-102	3.6	198
86	On the collective network of ionic liquid/water mixtures. I. Orientational structure. <i>Journal of Chemical Physics</i> , 2007 , 127, 234503	3.9	114
85	On the computation and contribution of conductivity in molecular ionic liquids. <i>Journal of Chemical Physics</i> , 2008 , 128, 134501	3.9	100
84	Simulation studies of ionic liquids: orientational correlations and static dielectric properties. <i>Journal of Chemical Physics</i> , 2006 , 125, 244506	3.9	91
83	Collective rotational dynamics in ionic liquids: a computational and experimental study of 1-butyl-3-methyl-imidazolium tetrafluoroborate. <i>Journal of Chemical Physics</i> , 2007 , 126, 084511	3.9	87
82	Proteins in Ionic Liquids: Current Status of Experiments and Simulations. <i>Topics in Current Chemistry</i> , 2017 , 375, 25	7.2	86
81	Intramolecular vibrational energy redistribution in bridged azulene-anthracene compounds: ballistic energy transport through molecular chains. <i>Journal of Chemical Physics</i> , 2004 , 121, 1754-64	3.9	84
80	On the collective network of ionic liquid/water mixtures. II. Decomposition and interpretation of dielectric spectra. <i>Journal of Chemical Physics</i> , 2008 , 129, 184501	3.9	83
79	Simulating polarizable molecular ionic liquids with Drude oscillators. <i>Journal of Chemical Physics</i> , 2010 , 133, 154511	3.9	77
78	Micellar catalysis in aqueous-ionic liquid systems. <i>Chemical Communications</i> , 2012 , 48, 5013-5	5.8	69
77	Simulation studies of the protein-water interface. I. Properties at the molecular resolution. <i>Journal of Chemical Physics</i> , 2006 , 124, 234907	3.9	66
76	Surface-active ionic liquids in micellar catalysis: impact of anion selection on reaction rates in nucleophilic substitutions. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 13375-84	3.6	59
75	Computational studies of ionic liquids: size does matter and time too. <i>Journal of Chemical Physics</i> , 2012 , 137, 094501	3.9	58
74	Polarisabilities of alkylimidazolium ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 2703-11	3.6	57
73	On the dielectric conductivity of molecular ionic liquids. <i>Journal of Chemical Physics</i> , 2009 , 131, 114504	3.9	53
72	Alchemical free energy calculations and multiple conformational substates. <i>Journal of Chemical Physics</i> , 2005 , 122, 84109	3.9	51

71	Collective translational motions and cage relaxations in molecular ionic liquids. <i>Journal of Chemical Physics</i> , 2011 , 135, 024502	3.9	51
70	The influence of electrostatic forces on the structure and dynamics of molecular ionic liquids. <i>Journal of Chemical Physics</i> , 2008 , 128, 224503	3.9	48
69	Impact of anisotropy on the structure and dynamics of ionic liquids: a computational study of 1-butyl-3-methyl-imidazolium trifluoroacetate. <i>Journal of Chemical Physics</i> , 2007 , 127, 044505	3.9	47
68	On the collective network of ionic liquid/water mixtures. III. Structural analysis of ionic liquids on the basis of Voronoi decomposition. <i>Journal of Chemical Physics</i> , 2009 , 130, 194503	3.9	46
67	Using fit functions in computational dielectric spectroscopy. <i>Journal of Chemical Physics</i> , 2010 , 132, 244109	3.9	45
66	Hydrated Ionic Liquids with and without Solute: The Influence of Water Content and Protein Solutes. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 3911-28	6.4	43
65	Solvation studies of a zinc finger protein in hydrated ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 6955-69	3.6	43
64	Exploring ionic liquid/biomass interactions: towards the improved isolation of shikimic acid from star anise pods. <i>RSC Advances</i> , 2013 , 3, 26010	3.7	41
63	Dielectric and terahertz spectroscopy of polarizable and nonpolarizable water models: a comparative study. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 1539-47	2.8	40
62	The influence of polarizability on the dielectric spectrum of the ionic liquid 1-ethyl-3-methylimidazolium triflate. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 12240-8	3.6	39
61	Simulation studies of the protein-water interface. II. Properties at the mesoscopic resolution. <i>Journal of Chemical Physics</i> , 2006 , 124, 234908	3.9	36
60	Relaxation of Voronoi shells in hydrated molecular ionic liquids. <i>Journal of Chemical Physics</i> , 2009 , 131, 174509	3.9	33
59	Intramolecular vibrational redistribution and energy relaxation in solution: A molecular dynamics approach. <i>Physical Chemistry Chemical Physics</i> , 2002 , 4, 271-278	3.6	32
58	Quantum mechanical determination of atomic polarizabilities of ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 10992-10996	3.6	30
57	Pair dynamics and the intermolecular nuclear Overhauser effect (NOE) in liquids analysed by simulation and model theories: application to an ionic liquid. <i>Journal of Chemical Physics</i> , 2014 , 140, 184503	3.9	28
56	Additive polarizabilities in ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 1665-70	3.6	27
55	Comparing induced point-dipoles and Drude oscillators. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 14297-306	3.6	27
54	Polarization effects on the solvation dynamics of coumarin C153 in ionic liquids: components and their cross-correlations. <i>Journal of Chemical Physics</i> , 2013 , 138, 204504	3.9	27

53	Basic chiral ionic liquids: A novel strategy for acid-free organocatalysis. <i>Catalysis Today</i> , 2013 , 200, 80-86	5.3	26
52	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
51	Communication: Solvation and dielectric response in ionic liquids--conductivity extension of the continuum model. <i>Journal of Chemical Physics</i> , 2013 , 138, 111102	3.9	22
50	Molecular dynamics simulation of heat conduction through a molecular chain. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 14039-51	2.8	22
49	Molecular dynamics analysis of the effect of electronic polarization on the structure and single-particle dynamics of mixtures of ionic liquids and lithium salts. <i>Journal of Chemical Physics</i> , 2016 , 145, 204507	3.9	22
48	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
47	Dielectric spectra of ionic liquids and their conversion to solvation dynamics: a detailed computational analysis of polarizable systems. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 10999-1009	3.6	18
46	Evaluating excited state atomic polarizabilities of chromophores. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 8554-8563	3.6	17
45	Computational analysis of the solvation of coffee ingredients in aqueous ionic liquid mixtures. <i>RSC Advances</i> , 2017 , 7, 3495-3504	3.7	15
44	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
43	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
42	Amino alcohol-derived chiral ionic liquids: structural investigations toward chiral recognition. <i>Tetrahedron: Asymmetry</i> , 2015 , 26, 1069-1082		14
41	Intrinsic Structure of the Interface of Partially Miscible Fluids: An Application to Ionic Liquids. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 28448-28461	3.8	13
40	A shell-resolved analysis of preferential solvation of coffee ingredients in aqueous mixtures of the ionic liquid 1-ethyl-3-methylimidazolium acetate. <i>Journal of Chemical Physics</i> , 2018 , 148, 193819	3.9	13
39	Langevin behavior of the dielectric decrement in ionic liquid water mixtures. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 15106-15117	3.6	13
38	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
37	The effect of Thole functions on the simulation of ionic liquids with point induced dipoles at various densities. <i>Journal of Chemical Physics</i> , 2013 , 138, 204119	3.9	12
36	Additive polarizabilities of halides in ionic liquids and organic solvents. <i>Journal of Chemical Physics</i> , 2018 , 149, 044302	3.9	11

35	On the collective network of ionic liquid/water mixtures. IV. Kinetic and rotational depolarization. <i>Journal of Chemical Physics</i> , 2014 , 140, 204505	3.9	11
34	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
33	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
32	Orientalional alignment of amyloidogenic proteins in pre-aggregated solutions. <i>Physical Review Letters</i> , 2015 , 114, 128101	7.4	10
31	Computational solvation analysis of biomolecules in aqueous ionic liquid mixtures : From large flexible proteins to small rigid drugs. <i>Biophysical Reviews</i> , 2018 , 10, 825-840	3.7	10
30	Polarizable MD simulations of ionic liquids: How does additional charge transfer change the dynamics?. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 467-477	3.6	10
29	Computational solvation dynamics of oxyquinolinium betaine linked to trehalose. <i>Journal of Chemical Physics</i> , 2016 , 145, 164507	3.9	10
28	Ion-Tagged Chiral Ligands for Asymmetric Transfer Hydrogenations in Aqueous Medium. <i>ACS Sustainable Chemistry and Engineering</i> , 2019 , 7, 3414-3423	8.3	10
27	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
26	Proteins in Ionic Liquids: Current Status of Experiments and Simulations. <i>Topics in Current Chemistry Collections</i> , 2017 , 127-152	1.8	9
25	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
24	Polarizable molecular dynamics simulations of ionic liquids: Influence of temperature control. <i>Journal of Chemical Physics</i> , 2020 , 152, 094105	3.9	7
23	Selective Hydrogenation of Aldehydes Using a Well-Defined Fe(II) PNP Pincer Complex in Biphasic Medium. <i>ChemCatChem</i> , 2018 , 10, 4386-4394	5.2	7
22	Surface-Active Ionic Liquids in Catalytic Water Splitting. <i>Australian Journal of Chemistry</i> , 2019 , 72, 34	1.2	7
21	Surface-active ionic liquids: A review. <i>Journal of Molecular Liquids</i> , 2021 , 347, 118160	6	7
20	The physical significance of the Kamlet-Taft * parameter of ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 1616-1626	3.6	7
19	Molecular dynamics simulation of aqueous 1-dodecyl-3-methylimidazolium chloride: Emerging micelles. <i>Journal of Molecular Liquids</i> , 2018 , 272, 766-777	6	7
18	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

17	Computational Dielectric Spectroscopy of Charged, Dipolar Systems 2010 , 279-321		4
16	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
15	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
14	Computational analysis of conductivity contributions in an ionic liquid mixture of 1-ethyl-3-methylimidazolium dicyanamide and tetrafluoroborate. <i>Journal of Molecular Liquids</i> , 2019 , 288, 110993	6	3
13	Quantum Yields for the Photodissociation of Iodine in Compressed Liquids and Supercritical Fluids. <i>Zeitschrift Fur Physikalische Chemie</i> , 2001 , 215,	3.1	3
12	Charged, dipolar soft matter systems from a combined microscopic-mesoscopic viewpoint. <i>Journal of Physics Condensed Matter</i> , 2016 , 28, 344008	1.8	2
11	Non-additive electronic polarizabilities of ionic liquids: Charge delocalization effects. <i>Journal of Molecular Liquids</i> , 2021 , 346, 117099	6	2
10	Comparison between ab initio and polarizable molecular dynamics simulations of 1-butyl-3-methylimidazolium tetrafluoroborate and chloride in water. <i>Journal of Molecular Liquids</i> , 2021 , 337, 116521	6	2
9	General review of ionic liquids and their properties 2016 , 1-23		1
8	The influence of the cation structure on the basicity-related polarity of ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 26750-26760	3.6	1
7	Proteins in Ionic Liquids: Current Status of Experiments and Simulations 2017 , 375, 1		1
6	Computational solvation dynamics: Implementation, application, and validation. <i>Annual Reports in Computational Chemistry</i> , 2020 , 93-154	1.8	1
5	Enantiomerization of Axially Chiral Biphenyls: Polarizable MD Simulations in Water and Butylmethylether. <i>International Journal of Molecular Sciences</i> , 2020 , 21,	6.3	1
4	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
3	The Intermolecular NOE Depends on Isotope Selection: Short Range vs Long Range Behavior. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 8658-8663	6.4	1
2	Grid Services for Parallel Molecular Dynamics with NAMD and CHARMM. <i>Lecture Notes in Computer Science</i> , 2008 , 1036-1051	0.9	0
1	Charge delocalization and hyperpolarizability in ionic liquids. <i>Journal of Molecular Liquids</i> , 2021 , 118153	6	0