Pavel Jungwirth

List of Publications by Year in Descending Order

321 papers	17,903 citations	72 h-index	120 g-index
348 ext. papers	19,356 ext. citations	6.1 avg, IF	6.98 L-index

#	Paper	IF	Citations
321	Electronic structure of the solvated benzene radical anion.. *Journal of Chemical Physics*, **2022**, 156, 014501	3.9	1
320	Heavy Water Models for Classical Molecular Dynamics: Effective Inclusion of Nuclear Quantum Effects. *Journal of Physical Chemistry B*, **2021**, 125, 4514-4519	3.4	3
319	Sweet taste of heavy water. *Communications Biology*, **2021**, 4, 440	6.7	8
318	Benzene Radical Anion Microsolvated in Ammonia Clusters: Modeling the Transition from an Unbound Resonance to a Bound Species. *Journal of Physical Chemistry A*, **2021**, 125, 5811-5818	2.8	3
317	Resolving the Equal Number Density Puzzle: Molecular Picture from Simulations of LiCl(aq) and NaCl(aq). *Journal of Physical Chemistry B*, **2021**, 125, 3153-3162	3.4	2
316	Spectroscopic evidence for a gold-coloured metallic water solution. *Nature*, **2021**, 595, 673-676	50.4	2
315	Anisotropic diffusion of membrane proteins at experimental timescales. *Journal of Chemical Physics* , **2021**, 155, 015102	3.9	1
314	The glycine arginine-rich domain of the RNA-binding protein nucleolin regulates its subcellular localization. *EMBO Journal*, **2021**, 40, e107158	13	4
313	Photoelectron spectra of alkali metal-ammonia microjets: From blue electrolyte to bronze metal. *Science*, **2020**, 368, 1086-1091	33.3	26
312	Benzene Radical Anion in the Context of the Birch Reduction: When Solvation Is the Key. *Journal of Physical Chemistry Letters*, **2020**, 11, 6032-6038	6.4	6
311	Simulation of Raman and Raman optical activity of saccharides in solution. *Physical Chemistry Chemical Physics*, **2020**, 22, 1983-1993	3.6	12
310	Improved Cation Binding to Lipid Bilayers with Negatively Charged POPS by Effective Inclusion of Electronic Polarization. *Journal of Chemical Theory and Computation*, **2020**, 16, 738-748	6.4	15
309	Binding of divalent cations to acetate: molecular simulations guided by Raman spectroscopy. *Physical Chemistry Chemical Physics*, **2020**, 22, 24014-24027	3.6	16
308	Obtaining 3D Atomistic Structure of Saccharides from Raman/ROA/NMR Spectroscopic Techniques. *Biophysical Journal*, **2020**, 118, 298a	2.9	2
307	A practical guide to biologically relevant molecular simulations with charge scaling for electronic polarization. *Journal of Chemical Physics*, **2020**, 153, 050901	3.9	27
306	Tail-Oxidized Cholesterol Enhances Membrane Permeability for Small Solutes. *Langmuir*, **2020**, 36, 10438-10447	3.7	6
305	Deeply cooled and temperature controlled microjets: Liquid ammonia solutions released into vacuum for analysis by photoelectron spectroscopy. *Review of Scientific Instruments*, **2020**, 91, 043101	1.7	6

304	Valence and Core-Level X-ray Photoelectron Spectroscopy of a Liquid Ammonia Microjet. *Journal of the American Chemical Society*, **2019**, 141, 1838-1841	16.4	16
303	Quantifying the Strength of a Salt Bridge by Neutron Scattering and Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2019**, 10, 3254-3259	6.4	11
302	The Periodic Table. *Journal of Physical Chemistry A*, **2019**, 123, 5837-5848	2.8	1
301	The JPC Periodic Table. *Journal of Physical Chemistry C*, **2019**, 123, 17063-17074	3.8	1
300	The JPC Periodic Table. *Journal of Physical Chemistry Letters*, **2019**, 10, 4051-4062	6.4	1
299	Charge Scaling Manifesto: A Way of Reconciling the Inherently Macroscopic and Microscopic Natures of Molecular Simulations. *Journal of Physical Chemistry Letters*, **2019**, 10, 7531-7536	6.4	44
298	Structure and Dynamics of the Hydration Shell: Spatially Decomposed Time Correlation Approach. *Journal of Chemical Theory and Computation*, **2019**, 15, 803-812	6.4	8
297	Calcium ions in aqueous solutions: Accurate force field description aided by ab initio molecular dynamics and neutron scattering. *Journal of Chemical Physics*, **2018**, 148, 222813	3.9	51
296	Ion-Induced Long-Range Orientational Correlations in Water: Strong or Weak, Physiologically Relevant or Unimportant, and Unique to Water or Not?. *Journal of Physical Chemistry Letters*, **2018**, 9, 2056-2057	6.4	12
295	Bobbing of Oxysterols: Molecular Mechanism for Translocation of Tail-Oxidized Sterols through Biological Membranes. *Journal of Physical Chemistry Letters*, **2018**, 9, 1118-1123	6.4	18
294	Binding of Divalent Cations to Insulin: Capillary Electrophoresis and Molecular Simulations. *Journal of Physical Chemistry B*, **2018**, 122, 5640-5648	3.4	27
293	Accurate Binding of Sodium and Calcium to a POPC Bilayer by Effective Inclusion of Electronic Polarization. *Journal of Physical Chemistry B*, **2018**, 122, 4546-4557	3.4	56
292	Calcium Sensing by Recoverin: Effect of Protein Conformation on Ion Affinity. *Journal of Physical Chemistry Letters*, **2018**, 9, 1613-1619	6.4	11
291	Anomalous surface behavior of hydrated guanidinium ions due to ion pairing. *Journal of Chemical Physics*, **2018**, 148, 144508	3.9	10
290	Water dynamics in concentrated electrolytes: Local ion effect on hydrogen-bond jumps rather than collective coupling to ion clusters. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E4953-E4954	11.5	6
289	Hydration and Ion Pairing in Aqueous Mg and Zn Solutions: Force-Field Description Aided by Neutron Scattering Experiments and Ab Initio Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2018**, 122, 3296-3306	3.4	54
288	Arginine-rich cell-penetrating peptides induce membrane multilamellarity and subsequently enter via formation of a fusion pore. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 11923-11928	11.5	90
287	Can Arginine Inhibit Insulin Aggregation? A Combined Protein Crystallography, Capillary Electrophoresis, and Molecular Simulation Study. *Journal of Physical Chemistry B*, **2018**, 122, 10069-10078	3.4	21

286	Arginine "Magic": Guanidinium Like-Charge Ion Pairing from Aqueous Salts to Cell Penetrating Peptides. *Accounts of Chemical Research*, **2018**, 51, 1455-1464	24.3	80
285	Distributions of therapeutically promising neurosteroids in cellular membranes. *Chemistry and Physics of Lipids*, **2017**, 203, 78-86	3.7	2
284	Increased Binding of Calcium Ions at Positively Curved Phospholipid Membranes. *Journal of Physical Chemistry Letters*, **2017**, 8, 518-523	6.4	20
283	Beyond the Hofmeister Series: Ion-Specific Effects on Proteins and Their Biological Functions. *Journal of Physical Chemistry B*, **2017**, 121, 1997-2014	3.4	318
282	Calcium Directly Regulates Phosphatidylinositol 4,5-Bisphosphate Headgroup Conformation and Recognition. *Journal of the American Chemical Society*, **2017**, 139, 4019-4024	16.4	59
281	Two cations, two mechanisms: interactions of sodium and calcium with zwitterionic lipid membranes. *Chemical Communications*, **2017**, 53, 5380-5383	5.8	30
280	Size and Origins of Long-Range Orientational Water Correlations in Dilute Aqueous Salt Solutions. *Journal of Physical Chemistry Letters*, **2017**, 8, 2031-2035	6.4	20
279	Anomalous Protein-Protein Interactions in Multivalent Salt Solution. *Journal of Physical Chemistry B*, **2017**, 121, 3000-3006	3.4	18
278	Exploring Fluorescent Dyes at Biomimetic Interfaces with Second Harmonic Generation and Molecular Dynamics. *Langmuir*, **2017**, 33, 3373-3383	4	7
277	Computational and structural evidence for neurotransmitter-mediated modulation of the oligomeric states of human insulin in storage granules. *Journal of Biological Chemistry*, **2017**, 292, 8342-8355	5.4	12
276	Oxidation of Cholesterol Changes the Permeability of Lipid Membranes. *Biophysical Journal*, **2017**, 112, 377a	2.9	4
275	Guanidinium can both Cause and Prevent the Hydrophobic Collapse of Biomacromolecules. *Journal of the American Chemical Society*, **2017**, 139, 863-870	16.4	56
274	Self-association of a highly charged arginine-rich cell-penetrating peptide. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 11428-11433	11.5	38
273	Membrane Binding of Recoverin: From Mechanistic Understanding to Biological Functionality. *ACS Central Science*, **2017**, 3, 868-874	16.8	12
272	Changes in the hydration structure of imidazole upon protonation: Neutron scattering and molecular simulations. *Journal of Chemical Physics*, **2017**, 146, 185102	3.9	11
271	More than Virtual Reality: Important New Physical Insights in Simulations of Biomolecules and Synthetic Polymers. *Journal of Physical Chemistry B*, **2017**, 121, 6294	3.4	3
270	Accounting for Electronic Polarization Effects in Aqueous Sodium Chloride via Molecular Dynamics Aided by Neutron Scattering. *Journal of Physical Chemistry B*, **2016**, 120, 1454-60	3.4	79
269	Polyarginine Interacts More Strongly and Cooperatively than Polylysine with Phospholipid Bilayers. *Journal of Physical Chemistry B*, **2016**, 120, 9287-96	3.4	57

268	Dependence of the Rate of LiF Ion-Pairing on the Description of Molecular Interaction. *Journal of Physical Chemistry B*, **2016**, 120, 1749-58	3.4	12
267	Transmembrane Potential Modeling: Comparison between Methods of Constant Electric Field and Ion Imbalance. *Journal of Chemical Theory and Computation*, **2016**, 12, 2418-25	6.4	23
266	Guanidinium Pairing Facilitates Membrane Translocation. *Journal of Physical Chemistry B*, **2016**, 120, 143-53	3.4	18
265	The complex nature of calcium cation interactions with phospholipid bilayers. *Scientific Reports*, **2016**, 6, 38035	4.9	141
264	Innentitelbild: A Non-Exploding Alkali Metal Drop on Water: From Blue Solvated Electrons to Bursting Molten Hydroxide (Angew. Chem. 42/2016). *Angewandte Chemie*, **2016**, 128, 13108-13108	3.6	
263	A Non-Exploding Alkali Metal Drop on Water: From Blue Solvated Electrons to Bursting Molten Hydroxide. *Angewandte Chemie - International Edition*, **2016**, 55, 13019-13022	16.4	4
262	A Non-Exploding Alkali Metal Drop on Water: From Blue Solvated Electrons to Bursting Molten Hydroxide. *Angewandte Chemie*, **2016**, 128, 13213-13216	3.6	
261	Nonlinear Optical Properties of Fluorescent Dyes Allow for Accurate Determination of Their Molecular Orientations in Phospholipid Membranes. *Journal of Physical Chemistry B*, **2015**, 119, 9706-16	3.4	9
260	Hydration of hydroxyl and amino groups examined by molecular dynamics and neutron scattering. *Journal of Physical Chemistry B*, **2015**, 119, 6357-65	3.4	10
259	Biological Water or Rather Water in Biology?. *Journal of Physical Chemistry Letters*, **2015**, 6, 2449-51	6.4	57
258	Oxidation of cholesterol does not alter significantly its uptake into high-density lipoprotein particles. *Journal of Physical Chemistry B*, **2015**, 119, 4594-600	3.4	5
257	Exploring Ion-Ion Interactions in Aqueous Solutions by a Combination of Molecular Dynamics and Neutron Scattering. *Journal of Physical Chemistry Letters*, **2015**, 6, 1563-7	6.4	44
256	Modeling photoionization of aqueous DNA and its components. *Accounts of Chemical Research*, **2015**, 48, 1209-17	24.3	45
255	Membrane targeting of the yeast exocyst complex. *Biochimica Et Biophysica Acta - Biomembranes*, **2015**, 1848, 1481-9	3.8	36
254	Oxidation half-reaction of aqueous nucleosides and nucleotides via photoelectron spectroscopy augmented by ab initio calculations. *Journal of the American Chemical Society*, **2015**, 137, 201-9	16.4	57
253	Experimental determination and computational interpretation of biophysical properties of lipid bilayers enriched by cholesteryl hemisuccinate. *Biochimica Et Biophysica Acta - Biomembranes*, **2015**, 1848, 422-32	3.8	38
252	A comment on "pH and the surface tension of water" (J. K. Beattie, A. M. Djerdjev, A. Gray-Weale, N. Kallay, J. Lützenkirchen, T. Preočanin, A. Selmani, J. Colloid Interface Sci. 422 (2014) 54.). *Journal of Colloid and Interface Science*, **2015**, 448, 593	9.3	4
251	Cholesterol under oxidative stress-How lipid membranes sense oxidation as cholesterol is being replaced by oxysterols. *Free Radical Biology and Medicine*, **2015**, 84, 30-41	7.8	45

250	Coulomb explosion during the early stages of the reaction of alkali metals with water. *Nature Chemistry*, **2015**, 7, 250-4	17.6	67
249	Beyond Hofmeister. *Nature Chemistry*, **2014**, 6, 261-3	17.6	301
248	Accurate determination of the orientational distribution of a fluorescent molecule in a phospholipid membrane. *Journal of Physical Chemistry B*, **2014**, 118, 855-63	3.4	22
247	How well does cholesteryl hemisuccinate mimic cholesterol in saturated phospholipid bilayers?. *Journal of Molecular Modeling*, **2014**, 20, 2121	2	33
246	Surface behavior of hydrated guanidinium and ammonium ions: a comparative study by photoelectron spectroscopy and molecular dynamics. *Journal of Physical Chemistry B*, **2014**, 118, 7119-27	3.4	23
245	Hydration of the chloride ion in concentrated aqueous solutions using neutron scattering and molecular dynamics. *Molecular Physics*, **2014**, 112, 1230-1240	1.7	34
244	Single lipid extraction: the anchoring strength of cholesterol in liquid-ordered and liquid-disordered phases. *Biophysical Journal*, **2014**, 107, 1167-1175	2.9	23
243	Aqueous Cation-Amide Binding: Free Energies and IR Spectral Signatures by Ab Initio Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2014**, 5, 2235-40	6.4	32
242	Accurate description of calcium solvation in concentrated aqueous solutions. *Journal of Physical Chemistry B*, **2014**, 118, 7902-9	3.4	104
241	Optical spectroscopy of the bulk and interfacial hydrated electron from ab initio calculations. *Journal of Physical Chemistry A*, **2014**, 118, 7507-15	2.8	48
240	Direct observation of the collapse of the delocalized excess electron in water. *Nature Chemistry*, **2014**, 6, 697-701	17.6	48
239	Charges at Aqueous Interfaces: Development of Computational Approaches in Direct Contact with Experiment. *Advances in Chemical Physics*, **2014**, 69-96		1
238	Calcium Binding to Calmodulin by Molecular Dynamics with Effective Polarization. *Journal of Physical Chemistry Letters*, **2014**, 5, 3964-9	6.4	51
237	Electrophoretic mobilities of neutral analytes and electroosmotic flow markers in aqueous solutions of Hofmeister salts. *Electrophoresis*, **2014**, 35, 617-24	3.6	7
236	Does fluoride disrupt hydrogen bond network in cationic lipid bilayer? Time-dependent fluorescence shift of Laurdan and molecular dynamics simulations. *Journal of Chemical Physics*, **2014**, 141, 22D516	3.9	3
235	Specific potassium ion interactions facilitate homocysteine binding to betaine-homocysteine S-methyltransferase. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 2552-64	4.2	6
234	DNA lesion can facilitate base ionization: vertical ionization energies of aqueous 8-oxoguanine and its nucleoside and nucleotide. *Journal of Physical Chemistry B*, **2014**, 118, 13833-7	3.4	10
233	Mechanisms of acceleration and retardation of water dynamics by ions. *Journal of the American Chemical Society*, **2013**, 135, 11824-31	16.4	166

232	Unexpectedly Small Effect of the DNA Environment on Vertical Ionization Energies of Aqueous Nucleobases. *Journal of Physical Chemistry Letters*, **2013**, 4, 3766-3769	6.4	31
231	Embedded Cluster Models for Reactivity of the Hydrated Electron. *Zeitschrift Fur Physikalische Chemie*, **2013**, 227,	3.1	6
230	Ab Initio Molecular Dynamics Approach to a Quantitative Description of Ion Pairing in Water. *Journal of Physical Chemistry Letters*, **2013**, 4, 4177-4181	6.4	35
229	Effects of End Group Termination on Salting-Out Constants for Triglycine. *Journal of Physical Chemistry Letters*, **2013**, 4, 4069-4073	6.4	19
228	Aggregation of oligoarginines at phospholipid membranes: molecular dynamics simulations, time-dependent fluorescence shift, and biomimetic colorimetric assays. *Journal of Physical Chemistry B*, **2013**, 117, 11530-40	3.4	27
227	Electron at the Surface of Water: Dehydrated or Not?. *Journal of Physical Chemistry Letters*, **2013**, 4, 338-43	6.4	45
226	Ion pairing in aqueous lithium salt solutions with monovalent and divalent counter-anions. *Journal of Physical Chemistry A*, **2013**, 117, 11766-73	2.8	95
225	Cation-specific effects on enzymatic catalysis driven by interactions at the tunnel mouth. *Journal of Physical Chemistry B*, **2013**, 117, 6394-402	3.4	17
224	Reversal of the hofmeister series: specific ion effects on peptides. *Journal of Physical Chemistry B*, **2013**, 117, 8150-8	3.4	137
223	Aqueous guanidinium-carbonate interactions by molecular dynamics and neutron scattering: relevance to ion-protein interactions. *Journal of Physical Chemistry B*, **2013**, 117, 1844-8	3.4	30
222	Release of halide ions from the buried active site of the haloalkane dehalogenase LinB revealed by stopped-flow fluorescence analysis and free energy calculations. *Journal of Physical Chemistry B*, **2013**, 117, 14329-35	3.4	4
221	Correction to "Unraveling the Complex Nature of the Hydrated Electron". *Journal of Physical Chemistry Letters*, **2013**, 4, 603	6.4	3
220	Hofmeister Series of Ions: A Simple Theory of a Not So Simple Reality. *Journal of Physical Chemistry Letters*, **2013**, 4, 4258-9	6.4	11
219	Structure, dynamics, and reactivity of hydrated electrons by ab initio molecular dynamics. *Accounts of Chemical Research*, **2012**, 45, 23-32	24.3	77
218	Behavior of 4-hydroxynonenal in phospholipid membranes. *Journal of Physical Chemistry B*, **2012**, 116, 6411-5	3.4	27
217	Peptide salt bridge stability: from gas phase via microhydration to bulk water simulations. *Journal of Chemical Physics*, **2012**, 137, 185101	3.9	14
216	Accurate description of aqueous carbonate ions: an effective polarization model verified by neutron scattering. *Journal of Physical Chemistry B*, **2012**, 116, 8145-53	3.4	46
215	Semiclassical hybrid approach to condensed phase molecular dynamics: application to the I2Kr17 cluster. *Journal of Physical Chemistry A*, **2012**, 116, 11199-210	2.8	18

214	Affine-response model of molecular solvation of ions: Accurate predictions of asymmetric charging free energies. *Journal of Chemical Physics*, **2012**, 137, 124101	3.9	35
213	Solvation and ion-pairing properties of the aqueous sulfate anion: explicit versus effective electronic polarization. *Physical Chemistry Chemical Physics*, **2012**, 14, 10248-57	3.6	62
212	Structure, dynamics, and hydration of POPC/POPS bilayers suspended in NaCl, KCl, and CsCl solutions. *Biochimica Et Biophysica Acta - Biomembranes*, **2012**, 1818, 609-16	3.8	86
211	Biophysics of lipid bilayers containing oxidatively modified phospholipids: insights from fluorescence and EPR experiments and from MD simulations. *Biochimica Et Biophysica Acta - Biomembranes*, **2012**, 1818, 2388-402	3.8	92
210	Lipid hydration and mobility: an interplay between fluorescence solvent relaxation experiments and molecular dynamics simulations. *Biochimie*, **2012**, 94, 26-32	4.6	60
209	Unraveling the Complex Nature of the Hydrated Electron. *Journal of Physical Chemistry Letters*, **2012**, 3, 3071-5	6.4	99
208	Charge Transfer between Water Molecules As the Possible Origin of the Observed Charging at the Surface of Pure Water. *Journal of Physical Chemistry Letters*, **2012**, 3, 107-111	6.4	86
207	Like-Charge Ion Pairing in Water: An Ab Initio Molecular Dynamics Study of Aqueous Guanidinium Cations. *Journal of Physical Chemistry Letters*, **2012**, 3, 2021-2024	6.4	49
206	Transforming anion instability into stability: contrasting photoionization of three protonation forms of the phosphate ion upon moving into water. *Journal of Physical Chemistry B*, **2012**, 116, 13254-64	3.4	40
205	Ions at Hydrophobic Aqueous Interfaces: Molecular Dynamics with Effective Polarization. *Journal of Physical Chemistry Letters*, **2012**, 3, 2087-2091	6.4	76
204	Molecular mechanisms of ion-specific effects on proteins. *Journal of the American Chemical Society*, **2012**, 134, 10039-46	16.4	217
203	Counterion condensation in short cationic peptides: limiting mobilities beyond the Onsager-Fuoss theory. *Electrophoresis*, **2012**, 33, 981-9	3.6	12
202	Overcharging in biological systems: reversal of electrophoretic mobility of aqueous polyaspartate by multivalent cations. *Physical Review Letters*, **2012**, 108, 186101	7.4	47
201	Oxidized phosphatidylcholines facilitate phospholipid flip-flop in liposomes. *Biophysical Journal*, **2011**, 101, 1376-84	2.9	80
200	The orientation and charge of water at the hydrophobic oil droplet-water interface. *Journal of the American Chemical Society*, **2011**, 133, 10204-10	16.4	175
199	Ionization of purine tautomers in nucleobases, nucleosides, and nucleotides: from the gas phase to the aqueous environment. *Journal of Physical Chemistry B*, **2011**, 115, 1294-305	3.4	61
198	Like-charge guanidinium pairing from molecular dynamics and ab initio calculations. *Journal of Physical Chemistry A*, **2011**, 115, 11193-201	2.8	48
197	The effect of lipid oxidation on the water permeability of phospholipids bilayers. *Physical Chemistry Chemical Physics*, **2011**, 13, 17555-63	3.6	71

196	From a localized H3O radical to a delocalized H3O+ - solvent-separated pair by sequential hydration. *Physical Chemistry Chemical Physics*, **2011**, 13, 14003-9	3.6	16
195	Arrhenius analysis of anisotropic surface self-diffusion on the prismatic facet of ice. *Physical Chemistry Chemical Physics*, **2011**, 13, 19960-9	3.6	26
194	Internal structure, hygroscopic and reactive properties of mixed sodium methanesulfonate-sodium chloride particles. *Physical Chemistry Chemical Physics*, **2011**, 13, 11846-57	3.6	24
193	Microhydration of the magnesium(II) acetate cation in the gas phase. *Journal of Physical Chemistry A*, **2011**, 115, 6813-9	2.8	20
192	Complex ion effects on polypeptide conformational stability: chloride and sulfate salts of guanidinium and tetrapropylammonium. *Journal of the American Chemical Society*, **2011**, 133, 7300-3	16.4	31
191	Orientational dependence of the affinity of guanidinium ions to the water surface. *Journal of Physical Chemistry B*, **2011**, 115, 12521-6	3.4	38
190	Increased Propensity of Iaq for the Water Surface in Non-neutral Solutions: Implications for the Interfacial Behavior of H3Oaq+ and OHaq *Journal of Physical Chemistry Letters*, **2011**, 2, 972-976	6.4	17
189	Behavior of amyloid 1-16 at the air-water interface at varying pH by nonlinear spectroscopy and molecular dynamics simulations. *Journal of Physical Chemistry A*, **2011**, 115, 5873-80	2.8	7
188	Urea and guanidinium induced denaturation of a Trp-cage miniprotein. *Journal of Physical Chemistry B*, **2011**, 115, 8910-24	3.4	54
187	Guanidinium Cations Pair with Positively Charged Arginine Side Chains in Water. *Journal of Physical Chemistry Letters*, **2011**, 2, 1387-1389	6.4	44
186	Energetic origin of proton affinity to the air/water interface. *Journal of Physical Chemistry B*, **2011**, 115, 4745-51	3.4	37
185	Behavior of the Eigen form of hydronium at the air/water interface. *Journal of Physical Chemistry A*, **2011**, 115, 5881-6	2.8	29
184	Tributes to Victoria Buch. *Journal of Physical Chemistry A*, **2011**, 115, 5709-14	2.8	
183	Chasing charge localization and chemical reactivity following photoionization in liquid water. *Journal of Chemical Physics*, **2011**, 135, 224510	3.9	70
182	Interactions of molecular ions with model phospholipid membranes. *Collection of Czechoslovak Chemical Communications*, **2011**, 76, 695-711		5
181	Effects of micro-hydration in proton transfer from H2S NO+ complex to water: Ab initio and molecular dynamics study. *Collection of Czechoslovak Chemical Communications*, **2011**, 76, 585-603		1
180	Dynamics of electron localization in warm versus cold water clusters. *Physical Review Letters*, **2010**, 105, 043002	7.4	61
179	Hydrogen forms in water by proton transfer to a distorted electron. *Journal of Physical Chemistry B*, **2010**, 114, 915-20	3.4	32

178	Comment on "An explanation for the charge on water's surface" by A. Gray-Weale and J. K. Beattie, Phys. Chem. Chem. Phys., 2009, 11, 10994. *Physical Chemistry Chemical Physics*, **2010**, 12, 14362-3; discussion 14364-6	3.6	12
177	Electrons in Cold Water Clusters: An ab Initio Molecular Dynamics Study of Localization and Metastable States *Journal of Physical Chemistry C*, **2010**, 114, 20489-20495	3.8	34
176	Interfacial molecular organization at aqueous solution surfaces of atmospherically relevant dimethyl sulfoxide and methanesulfonic Acid using sum frequency spectroscopy and molecular dynamics simulation. *Journal of Physical Chemistry B*, **2010**, 114, 15546-53	3.4	32
175	Mechanism of interaction of monovalent ions with phosphatidylcholine lipid membranes. *Journal of Physical Chemistry B*, **2010**, 114, 9504-9	3.4	81
174	Reversal of Hofmeister ordering for pairing of NH4(+) vs alkylated ammonium cations with halide anions in water. *Journal of Physical Chemistry B*, **2010**, 114, 10843-52	3.4	57
173	Effect of association with sulfate on the electrophoretic mobility of polyarginine and polylysine. *Journal of Physical Chemistry B*, **2010**, 114, 11934-41	3.4	36
172	Attractive interactions between side chains of histidine-histidine and histidine-arginine-based cationic dipeptides in water. *Journal of Physical Chemistry B*, **2010**, 114, 8744-9	3.4	59
171	. *Journal of Physical Chemistry C*, **2010**, 114, 7831-7838	3.8	35
170	Ion specificity at the peptide bond: molecular dynamics simulations of N-methylacetamide in aqueous salt solutions. *Journal of Physical Chemistry B*, **2010**, 114, 1213-20	3.4	95
169	Oxidation changes physical properties of phospholipid bilayers: fluorescence spectroscopy and molecular simulations. *Langmuir*, **2010**, 26, 6140-4	4	95
168	Effect of Water Polarizability on the Properties of Solutions of Polyvalent Ions: Simulations of Aqueous Sodium Sulfate with Different Force Fields. *Journal of Chemical Theory and Computation*, **2010**, 6, 3233-40	6.4	69
167	The influence of concentration on the molecular surface structure of simple and mixed aqueous electrolytes. *Physical Chemistry Chemical Physics*, **2010**, 12, 10693-700	3.6	50
166	Specific interactions of ammonium functionalities in amino acids with aqueous fluoride and iodide. *Journal of Physical Chemistry B*, **2010**, 114, 13853-60	3.4	18
165	Dielectric Interpretation of Specificity of Ion Pairing in Water. *Journal of Physical Chemistry Letters*, **2010**, 1, 300-303	6.4	38
164	Photoelectron spectroscopy of liquid water and aqueous solution: Electron effective attenuation lengths and emission-angle anisotropy. *Journal of Electron Spectroscopy and Related Phenomena*, **2010**, 177, 60-70	1.7	149
163	Massive oxidation of phospholipid membranes leads to pore creation and bilayer disintegration. *Chemical Physics Letters*, **2010**, 486, 99-103	2.5	78
162	Characterization of the triple ion [(CH3)4N+PF6-(CH3)4N+] in the gas-phase. *Chemical Physics Letters*, **2010**, 490, 14-18	2.5	18
161	Large variations in the propensity of aqueous oxychlorine anions for the solution/vapor interface. *Journal of Chemical Physics*, **2009**, 131, 124706	3.9	23

160	Hofmeister series and specific interactions of charged headgroups with aqueous ions. *Advances in Colloid and Interface Science*, **2009**, 146, 42-7	14.3	332
159	Reply to comments on Frontiers Article Behavior of hydroxide at the water/vapor interface *Chemical Physics Letters*, **2009**, 481, 19-21	2.5	20
158	Czech bibliometric system fosters mediocre research. *Nature*, **2009**, 460, 1079	50.4	1
157	A chemist realizes that popularity is no measure of strength. *Nature*, **2009**, 460, 555	50.4	
156	Behavior of hydroxide at the water/vapor interface. *Chemical Physics Letters*, **2009**, 474, 241-247	2.5	101
155	Microsolvation of the acetate anion [CH3CO2-(H2O)n, n= 1]: A photoelectron spectroscopy and ab initio computational study. *Chemical Physics Letters*, **2009**, 477, 41-44	2.5	14
154	Effects of alkali cations and halide anions on the DOPC lipid membrane. *Journal of Physical Chemistry A*, **2009**, 113, 7235-43	2.8	133
153	Ion Binding to Biomolecules **2009**, 217-230		
152	Molecular Dynamics Study of Ice Vapor Interactions via the Quasi-Liquid Layer. *Journal of Physical Chemistry C*, **2009**, 113, 4597-4604	3.8	40
151	Ion-specific interactions between halides and basic amino acids in water. *Journal of Physical Chemistry A*, **2009**, 113, 1969-75	2.8	46
150	Specificity of ion-protein interactions: complementary and competitive effects of tetrapropylammonium, guanidinium, sulfate, and chloride ions. *Journal of Physical Chemistry B*, **2009**, 113, 3227-34	3.4	60
149	Ion specific effects of sodium and potassium on the catalytic activity of HIV-1 protease. *Physical Chemistry Chemical Physics*, **2009**, 11, 7599-604	3.6	35
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