Pavel Jungwirth

List of Publications by Citations

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	Specific ion effects at the air/water interface. *Chemical Reviews*, **2006**, 106, 1259-81	68.1	1093
320	Ions at the Air/Water Interface. *Journal of Physical Chemistry B*, **2002**, 106, 6361-6373	3.4	663
319	Molecular Structure of Salt Solutions: A New View of the Interface with Implications for Heterogeneous Atmospheric Chemistry. *Journal of Physical Chemistry B*, **2001**, 105, 10468-10472	3.4	586
318	Experiments and simulations of ion-enhanced interfacial chemistry on aqueous NaCl aerosols. *Science*, **2000**, 288, 301-6	33.3	566
317	Unified molecular picture of the surfaces of aqueous acid, base, and salt solutions. *Journal of Physical Chemistry B*, **2005**, 109, 7617-23	3.4	374
316	Hofmeister series and specific interactions of charged headgroups with aqueous ions. *Advances in Colloid and Interface Science*, **2009**, 146, 42-7	14.3	332
315	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
314	Beyond Hofmeister. *Nature Chemistry*, **2014**, 6, 261-3	17.6	301
313	Water surface is acidic. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 7342-7	11.5	296
312	Ions at aqueous interfaces: from water surface to hydrated proteins. *Annual Review of Physical Chemistry*, **2008**, 59, 343-66	15.7	229
311	Biomolecular simulations of membranes: physical properties from different force fields. *Journal of Chemical Physics*, **2008**, 128, 125103	3.9	227
310	Molecular mechanisms of ion-specific effects on proteins. *Journal of the American Chemical Society*, **2012**, 134, 10039-46	16.4	217
309	Quantification and rationalization of the higher affinity of sodium over potassium to protein surfaces. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 15440-4	11.5	197
308	Propensity of soft ions for the air/water interface. *Current Opinion in Colloid and Interface Science*, **2004**, 9, 67-73	7.6	188
307	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
306	Air-liquid interfaces of aqueous solutions containing ammonium and sulfate: spectroscopic and molecular dynamics studies. *Journal of Physical Chemistry B*, **2005**, 109, 8861-72	3.4	175
305	Mechanisms of acceleration and retardation of water dynamics by ions. *Journal of the American Chemical Society*, **2013**, 135, 11824-31	16.4	166

304	Adsorption of Atmospherically Relevant Gases at the Air/Water Interface: Free Energy Profiles of Aqueous Solvation of N2, O2, O3, OH, H2O, HO2, and H2O2. *Journal of Physical Chemistry A*, **2004**, 108, 11573-11579	2.8	162
303	Enhanced concentration of polarizable anions at the liquid water surface: SHG spectroscopy and MD simulations of sodium thiocyanate [corrected]. *Journal of Physical Chemistry B*, **2005**, 109, 10915-21	3.4	160
302	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
301	The complex nature of calcium cation interactions with phospholipid bilayers. *Scientific Reports*, **2016**, 6, 38035	4.9	141
300	Autoionization at the surface of neat water: is the top layer pH neutral, basic, or acidic?. *Physical Chemistry Chemical Physics*, **2007**, 9, 4736-47	3.6	140
299	Reversal of the hofmeister series: specific ion effects on peptides. *Journal of Physical Chemistry B*, **2013**, 117, 8150-8	3.4	137
298	Cation-specific interactions with carboxylate in amino acid and acetate aqueous solutions: X-ray absorption and ab initio calculations. *Journal of Physical Chemistry B*, **2008**, 112, 12567-70	3.4	136
297	Surface solvation of halogen anions in water clusters: An ab initio molecular dynamics study of the Cl(H2O)6 complex. *Journal of Chemical Physics*, **2001**, 114, 7036-7044	3.9	136
296	Effects of alkali cations and halide anions on the DOPC lipid membrane. *Journal of Physical Chemistry A*, **2009**, 113, 7235-43	2.8	133
295	Chloride Anion on Aqueous Clusters, at the Air Water Interface, and in Liquid Water: Solvent Effects on Cl-Polarizability. *Journal of Physical Chemistry A*, **2002**, 106, 379-383	2.8	131
294	The molecular origin of like-charge arginine-arginine pairing in water. *Journal of Physical Chemistry B*, **2009**, 113, 9041-5	3.4	123
293	Specific ion effects at protein surfaces: a molecular dynamics study of bovine pancreatic trypsin inhibitor and horseradish peroxidase in selected salt solutions. *Journal of Physical Chemistry B*, **2006**, 110, 7036-43	3.4	119
292	Polarizability of the nitrate anion and its solvation at the air/water interface. *Physical Chemistry Chemical Physics*, **2003**, 5, 3752	3.6	119
291	Specific ion binding to nonpolar surface patches of proteins. *Journal of the American Chemical Society*, **2008**, 130, 11582-3	16.4	114
290	Brine rejection from freezing salt solutions: a molecular dynamics study. *Physical Review Letters*, **2005**, 95, 148501	7.4	114
289	Ionization energies of aqueous nucleic acids: photoelectron spectroscopy of pyrimidine nucleosides and ab initio calculations. *Journal of the American Chemical Society*, **2009**, 131, 6460-7	16.4	113
288	Excited States of Iodide Anions in Water: A Comparison of the Electronic Structure in Clusters and in Bulk Solution. *Journal of Physical Chemistry A*, **2002**, 106, 1286-1298	2.8	112
287	Surface Effects on Aqueous Ionic Solvation: A Molecular Dynamics Simulation Study of NaCl at the Air/Water Interface from Infinite Dilution to Saturation. *Journal of Physical Chemistry B*, **2000**, 104, 7702-7706	3.4	109

286	Accurate description of calcium solvation in concentrated aqueous solutions. *Journal of Physical Chemistry B*, **2014**, 118, 7902-9	3.4	104
285	Behavior of hydroxide at the water/vapor interface. *Chemical Physics Letters*, **2009**, 474, 241-247	2.5	101
284	Uracil Dimer: Potential Energy and Free Energy Surfaces. Ab Initio beyond Hartree−Fock and Empirical Potential Studies. *Journal of Physical Chemistry A*, **1998**, 102, 6921-6926	2.8	100
283	Unraveling the Complex Nature of the Hydrated Electron. *Journal of Physical Chemistry Letters*, **2012**, 3, 3071-5	6.4	99
282	Specific ion binding to macromolecules: effects of hydrophobicity and ion pairing. *Langmuir*, **2008**, 24, 3387-91	4	99
281	Homogeneous freezing of water starts in the subsurface. *Journal of Physical Chemistry B*, **2006**, 110, 18126-9	3.4	99
280	Electron binding energies of aqueous alkali and halide ions: EUV photoelectron spectroscopy of liquid solutions and combined ab initio and molecular dynamics calculations. *Journal of the American Chemical Society*, **2005**, 127, 7203-14	16.4	98
279	Structure and vibrational spectroscopy of salt water/air interfaces: predictions from classical molecular dynamics simulations. *Journal of Physical Chemistry B*, **2005**, 109, 7934-40	3.4	96
278	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
277	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
276	Oxidation changes physical properties of phospholipid bilayers: fluorescence spectroscopy and molecular simulations. *Langmuir*, **2010**, 26, 6140-4	4	95
275	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
274	Monitoring Ice Nucleation in Pure and Salty Water via High-Speed Imaging and Computer Simulations. *Journal of Physical Chemistry C*, **2008**, 112, 7631-7636	3.8	90
273	Polarizability and aqueous solvation of the sulfate dianion. *Chemical Physics Letters*, **2003**, 367, 704-710	2.5	90
272	How Many Waters Are Necessary To Dissolve a Rock Salt Molecule?. *Journal of Physical Chemistry A*, **2000**, 104, 145-148	2.8	90
271	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
270	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
269	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

268	Electron binding energies of hydrated H3O+ and OH-: photoelectron spectroscopy of aqueous acid and base solutions combined with electronic structure calculations. *Journal of the American Chemical Society*, **2006**, 128, 3864-5	16.4	84
267	Impact, Trapping, and Accommodation of Hydroxyl Radical and Ozone at Aqueous Salt Aerosol Surfaces. A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2003**, 107, 12690-12699	3.4	84
266	Mechanism of interaction of monovalent ions with phosphatidylcholine lipid membranes. *Journal of Physical Chemistry B*, **2010**, 114, 9504-9	3.4	81
265	Oxidized phosphatidylcholines facilitate phospholipid flip-flop in liposomes. *Biophysical Journal*, **2011**, 101, 1376-84	2.9	80
264	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
263	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
262	Massive oxidation of phospholipid membranes leads to pore creation and bilayer disintegration. *Chemical Physics Letters*, **2010**, 486, 99-103	2.5	78
261	Structure, dynamics, and reactivity of hydrated electrons by ab initio molecular dynamics. *Accounts of Chemical Research*, **2012**, 45, 23-32	24.3	77
260	Electronic structure of the water dimer cation. *Journal of Physical Chemistry A*, **2008**, 112, 6159-70	2.8	77
259	Ionization of imidazole in the gas phase, microhydrated environments, and in aqueous solution. *Journal of Physical Chemistry A*, **2008**, 112, 3499-505	2.8	77
258	Ions at Hydrophobic Aqueous Interfaces: Molecular Dynamics with Effective Polarization. *Journal of Physical Chemistry Letters*, **2012**, 3, 2087-2091	6.4	76
257	Ion partitioning at the liquid/vapor interface of a multicomponent alkali halide solution: a model for aqueous sea salt aerosols. *Journal of Physical Chemistry A*, **2008**, 112, 12378-84	2.8	76
256	Propensity for the air/water interface and ion pairing in magnesium acetate vs magnesium nitrate solutions: molecular dynamics simulations and surface tension measurements. *Journal of Physical Chemistry B*, **2006**, 110, 15939-44	3.4	75
255	Ion specific protein assembly and hydrophobic surface forces. *Physical Review Letters*, **2008**, 100, 258105	7.4	73
254	Spiers Memorial Lecture. Ions at aqueous interfaces. *Faraday Discussions*, **2009**, 141, 9-30; discussion 81-98	3.6	72
253	Ab initio molecular dynamics simulation of a medium-sized water cluster anion: from an interior to a surface-located excess electron via a delocalized state. *Journal of Physical Chemistry A*, **2008**, 112, 6125-33	2.8	72
252	Ion pairing as a possible clue for discriminating between sodium and potassium in biological and other complex environments. *Journal of Physical Chemistry B*, **2007**, 111, 14077-9	3.4	72
251	Molecular Structure of Surface-Active Salt Solutions: Photoelectron Spectroscopy and Molecular Dynamics Simulations of Aqueous Tetrabutylammonium Iodide *Journal of Physical Chemistry B*, **2004**, 108, 14558-14564	3.4	72

250	The effect of lipid oxidation on the water permeability of phospholipids bilayers. *Physical Chemistry Chemical Physics*, **2011**, 13, 17555-63	3.6	71
249	Chasing charge localization and chemical reactivity following photoionization in liquid water. *Journal of Chemical Physics*, **2011**, 135, 224510	3.9	70
248	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
247	Micro-hydration of the MgNO3+ cation in the gas phase. *ChemPhysChem*, **2007**, 8, 1629-39	3.2	69
246	Coulomb explosion during the early stages of the reaction of alkali metals with water. *Nature Chemistry*, **2015**, 7, 250-4	17.6	67
245	Hydronium and hydroxide at the interface between water and hydrophobic media. *Physical Chemistry Chemical Physics*, **2008**, 10, 4975-80	3.6	65
244	On the Convergence of the Physicochemical Properties of [n]Helicenes. *Journal of Physical Chemistry C*, **2007**, 111, 14948-14955	3.8	65
243	Molecular model of a cell plasma membrane with an asymmetric multicomponent composition: water permeation and ion effects. *Biophysical Journal*, **2009**, 96, 4493-501	2.9	63
242	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
241	Adsorption of polycyclic aromatic hydrocarbons at the air-water interface: molecular dynamics simulations and experimental atmospheric observations. *Physical Chemistry Chemical Physics*, **2006**, 8, 4461-7	3.6	62
240	Quantum Molecular Dynamics of Ultrafast Processes in Large Polyatomic Systems. *Chemical Reviews*, **1999**, 99, 1583-1606	68.1	62
239	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
238	Dynamics of electron localization in warm versus cold water clusters. *Physical Review Letters*, **2010**, 105, 043002	7.4	61
237	Lipid hydration and mobility: an interplay between fluorescence solvent relaxation experiments and molecular dynamics simulations. *Biochimie*, **2012**, 94, 26-32	4.6	60
236	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
235	Salt Crystallization from an Evaporating Aqueous Solution by Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2003**, 107, 8271-8274	3.4	60
234	Calcium Directly Regulates Phosphatidylinositol 4,5-Bisphosphate Headgroup Conformation and Recognition. *Journal of the American Chemical Society*, **2017**, 139, 4019-4024	16.4	59
233	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

232	Biological Water or Rather Water in Biology?. *Journal of Physical Chemistry Letters*, **2015**, 6, 2449-51	6.4	57
231	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
230	Polyarginine Interacts More Strongly and Cooperatively than Polylysine with Phospholipid Bilayers. *Journal of Physical Chemistry B*, **2016**, 120, 9287-96	3.4	57
229	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
228	Guanidinium can both Cause and Prevent the Hydrophobic Collapse of Biomacromolecules. *Journal of the American Chemical Society*, **2017**, 139, 863-870	16.4	56
227	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
226	Ultrasonic velocities, densities, viscosities, electrical conductivities, Raman spectra, and molecular dynamics simulations of aqueous solutions of Mg(OAc)2 and Mg(NO3)2: Hofmeister effects and ion pair formation. *Journal of Physical Chemistry B*, **2005**, 109, 24108-20	3.4	56
225	Aqueous solutions of ionic liquids: study of the solution/vapor interface using molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2008**, 10, 5765-75	3.6	55
224	Urea and guanidinium induced denaturation of a Trp-cage miniprotein. *Journal of Physical Chemistry B*, **2011**, 115, 8910-24	3.4	54
223	Quantum dynamics of large polyatomic systems using a classically based separable potential method. *Journal of Chemical Physics*, **1995**, 102, 6046-6056	3.9	54
222	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
221	Bulk versus interfacial aqueous solvation of dicarboxylate dianions. *Journal of the American Chemical Society*, **2004**, 126, 11691-8	16.4	53
220	Molecular dynamics simulations of freezing of water and salt solutions. *Journal of Molecular Liquids*, **2007**, 134, 64-70	6	52
219	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
218	Calcium Binding to Calmodulin by Molecular Dynamics with Effective Polarization. *Journal of Physical Chemistry Letters*, **2014**, 5, 3964-9	6.4	51
217	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
216	The C4H8.bul.+ potential energy surface. 2. The (C2H4)2.bul.+ complex cation and its reaction to the radical cations of cyclobutane and 1-butene. *Journal of the American Chemical Society*, **1993**, 115, 5783-5789	16.4	50
215	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

214	Simulated surface potentials at the vapor-water interface for the KCl aqueous electrolyte solution. *Journal of Chemical Physics*, **2006**, 125, 24706	3.9	49
213	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
212	Direct observation of the collapse of the delocalized excess electron in water. *Nature Chemistry*, **2014**, 6, 697-701	17.6	48
211	Like-charge guanidinium pairing from molecular dynamics and ab initio calculations. *Journal of Physical Chemistry A*, **2011**, 115, 11193-201	2.8	48
210	Water Structuring and Hydroxide Ion Binding at the Interface between Water and Hydrophobic Walls of Varying Rigidity and van der Waals Interactions. *Journal of Physical Chemistry C*, **2008**, 112, 7689-7692	3.8	48
209	Propensity of Formate, Acetate, Benzoate, and Phenolate for the Aqueous Solution/Vapor Interface: Surface Tension Measurements and Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2007**, 111, 8242-8247	3.8	48
208	Overcharging in biological systems: reversal of electrophoretic mobility of aqueous polyaspartate by multivalent cations. *Physical Review Letters*, **2012**, 108, 186101	7.4	47
207	Determination of the electron affinity of the acetyloxyl radical (CH3COO) by low-temperature anion photoelectron spectroscopy and ab initio calculations. *Journal of Physical Chemistry A*, **2006**, 110, 5047-50	2.8	47
206	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
205	Ion-specific interactions between halides and basic amino acids in water. *Journal of Physical Chemistry A*, **2009**, 113, 1969-75	2.8	46
204	The C4H8.bul.+ potential energy surface. 1. The cyclobutane radical cation. *Journal of the American Chemical Society*, **1993**, 115, 5776-5782	16.4	46
203	Modeling photoionization of aqueous DNA and its components. *Accounts of Chemical Research*, **2015**, 48, 1209-17	24.3	45
202	Electron at the Surface of Water: Dehydrated or Not?. *Journal of Physical Chemistry Letters*, **2013**, 4, 338-43	6.4	45
201	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
200	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
199	Guanidinium Cations Pair with Positively Charged Arginine Side Chains in Water. *Journal of Physical Chemistry Letters*, **2011**, 2, 1387-1389	6.4	44
198	A possible new molecular mechanism of thundercloud electrification. *Atmospheric Research*, **2005**, 76, 190-205	5.4	44
197	Surface segregation of dissolved salt ions. *Journal of Physical Chemistry B*, **2006**, 110, 11971-6	3.4	44

196	Solvation of the Azide Anion (N3-) in Water Clusters and Aqueous Interfaces: A Combined Investigation by Photoelectron Spectroscopy, Density Functional Calculations, and Molecular Dynamics Simulations *Journal of Physical Chemistry A*, **2004**, 108, 7820-7826	2.8	44
195	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
194	Electron Binding to Nucleic Acid Bases. Experimental and Theoretical Studies. A Review. *Collection of Czechoslovak Chemical Communications*, **2004**, 69, 1395-1428		42
193	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
192	Molecular Dynamics Study of Ice Vapor Interactions via the Quasi-Liquid Layer. *Journal of Physical Chemistry C*, **2009**, 113, 4597-4604	3.8	40
191	Patchy proteins, anions and the Hofmeister series. *Journal of Physics Condensed Matter*, **2008**, 20, 494218	1.8	40
190	Solvent-mediated folding of a doubly charged anion. *Journal of the American Chemical Society*, **2004** , 126, 876-83	16.4	39
189	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
188	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
187	Orientational dependence of the affinity of guanidinium ions to the water surface. *Journal of Physical Chemistry B*, **2011**, 115, 12521-6	3.4	38
186	Dielectric Interpretation of Specificity of Ion Pairing in Water. *Journal of Physical Chemistry Letters*, **2010**, 1, 300-303	6.4	38
185	Energetic origin of proton affinity to the air/water interface. *Journal of Physical Chemistry B*, **2011**, 115, 4745-51	3.4	37
184	Membrane targeting of the yeast exocyst complex. *Biochimica Et Biophysica Acta - Biomembranes*, **2015**, 1848, 1481-9	3.8	36
183	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
182	Response to Comment on Autoionization at the surface of neat water: is the top layer pH neutral, basic, or acidic? by J. K. Beattie, Phys. Chem. Chem. Phys., 2007, 9, DOI: 10.1039/b713702h. *Physical Chemistry Chemical Physics*, **2008**, 10, 332-333	3.6	36
181	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
180	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
179	. *Journal of Physical Chemistry C*, **2010**, 114, 7831-7838	3.8	35

178	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
177	Adsorption of aromatic hydrocarbons and ozone at environmental aqueous surfaces. *Journal of Physical Chemistry A*, **2008**, 112, 4942-50	2.8	35
176	Hydration of the chloride ion in concentrated aqueous solutions using neutron scattering and molecular dynamics. *Molecular Physics*, **2014**, 112, 1230-1240	1.7	34
175	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
174	Photolysis of hydrogen chloride embedded in the first argon solvation shell: Rotational control and quantum dynamics of photofragments. *Journal of Chemical Physics*, **1999**, 110, 6246-6256	3.9	34
173	How well does cholesteryl hemisuccinate mimic cholesterol in saturated phospholipid bilayers?. *Journal of Molecular Modeling*, **2014**, 20, 2121	2	33
172	Ab initio electronic structure of thymine anions. *Physical Chemistry Chemical Physics*, **2005**, 7, 840-5	3.6	33
171	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
170	Hydrogen forms in water by proton transfer to a distorted electron. *Journal of Physical Chemistry B*, **2010**, 114, 915-20	3.4	32
169	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
168	Ionization of aqueous cations: photoelectron spectroscopy and ab initio calculations of protonated imidazole. *Journal of Physical Chemistry B*, **2008**, 112, 7355-8	3.4	32
167	Quantum dynamics simulations of nonadiabatic processes in many-atom systems: Photoexcited Ba(Ar)10 and Ba(Ar)20 clusters. *Journal of Chemical Physics*, **1996**, 104, 5803-5814	3.9	32
166	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
165	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
164	Ultrafast quantum dynamics and resonance Raman spectroscopy of photoexcited I2(B) in large argon and xenon clusters. *Journal of Chemical Physics*, **1996**, 104, 9332-9339	3.9	31
163	Two cations, two mechanisms: interactions of sodium and calcium with zwitterionic lipid membranes. *Chemical Communications*, **2017**, 53, 5380-5383	5.8	30
162	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
161	Cluster model for the ionic product of water: accuracy and limitations of common density functional methods. *Journal of Physical Chemistry A*, **2006**, 110, 9194-9	2.8	30

160	Behavior of the Eigen form of hydronium at the air/water interface. *Journal of Physical Chemistry A*, **2011**, 115, 5881-6	2.8	29
159	Pickup and Photodissociation of Hydrogen Halides in Floppy Neon Clusters. *Journal of Physical Chemistry A*, **2003**, 107, 7743-7754	2.8	29
158	Effect of bromide on the interfacial structure of aqueous tetrabutylammonium iodide: Photoelectron spectroscopy and molecular dynamics simulations. *Chemical Physics Letters*, **2005**, 410, 222-227	2.5	29
157	Preference of cluster isomers as a result of quantum delocalization: Potential energy surfaces and intermolecular vibrational states of Ne?HBr, Ne?HI, and HI(Ar)n (n=1). *Journal of Chemical Physics*, **2001**, 114, 1539-1548	3.9	29
156	Time-dependent stokes shifts of fluorescent dyes in the hydrophobic backbone region of a phospholipid bilayer: combination of fluorescence spectroscopy and ab initio calculations. *Journal of Physical Chemistry B*, **2007**, 111, 5869-77	3.4	28
155	Anions of Alkali Halide Salts at Surfaces of Formamide Solutions: Concentration Depth Profiles and Surface Topography. *Journal of Physical Chemistry C*, **2007**, 111, 4379-4387	3.8	28
154	Binding of Divalent Cations to Insulin: Capillary Electrophoresis and Molecular Simulations. *Journal of Physical Chemistry B*, **2018**, 122, 5640-5648	3.4	27
153	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
152	Behavior of 4-hydroxynonenal in phospholipid membranes. *Journal of Physical Chemistry B*, **2012**, 116, 6411-5	3.4	27
151	Propensities of oxalic, citric, succinic, and maleic acids for the aqueous solution/vapour interface: Surface tension measurements and molecular dynamics simulations. *Chemical Physics Letters*, **2008**, 462, 217-221	2.5	27
150	Propensity of heavier halides for the water/vapor interface revisited using the Amoeba force field. *Chemical Physics Letters*, **2005**, 411, 70-74	2.5	27
149	A practical guide to biologically relevant molecular simulations with charge scaling for electronic polarization. *Journal of Chemical Physics*, **2020**, 153, 050901	3.9	27
148	Photoelectron spectra of alkali metal-ammonia microjets: From blue electrolyte to bronze metal. *Science*, **2020**, 368, 1086-1091	33.3	26
147	Arrhenius analysis of anisotropic surface self-diffusion on the prismatic facet of ice. *Physical Chemistry Chemical Physics*, **2011**, 13, 19960-9	3.6	26
146	Selected biologically relevant ions at the air/water interface: a comparative molecular dynamics study. *Biophysical Chemistry*, **2006**, 124, 238-42	3.5	25
145	Nonresonant ionization of oxygen molecules by femtosecond pulses: plasma dynamics studied by time-resolved terahertz spectroscopy. *Journal of Chemical Physics*, **2005**, 123, 104310	3.9	25
144	Photodissociation of HBr on the surface of Arn clusters at 193nm. *Chemical Physics*, **2005**, 315, 161-170	2.3	25
143	The parity non-conserving energy difference between enantiomers and a consequence of the CPT theorem for molecule-antimolecule pairs. *Chemical Physics Letters*, **1989**, 161, 502-506	2.5	25

142	Internal structure, hygroscopic and reactive properties of mixed sodium methanesulfonate-sodium chloride particles. *Physical Chemistry Chemical Physics*, **2011**, 13, 11846-57	3.6	24
141	HCl photodissociation on argon clusters: Effects of sequential solvation and librational preexcitation. *Journal of Chemical Physics*, **2000**, 112, 10761-10766	3.9	24
140	Size Effects on Photodissociation and Caging of Hydrogen Bromide Inside or on the Surface of Large Inert Clusters: From One to Three Icosahedral Argon Layers. *Journal of Physical Chemistry A*, **2000**, 104, 7793-7802	2.8	24
139	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
138	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
137	Single lipid extraction: the anchoring strength of cholesterol in liquid-ordered and liquid-disordered phases. *Biophysical Journal*, **2014**, 107, 1167-1175	2.9	23
136	Large variations in the propensity of aqueous oxychlorine anions for the solution/vapor interface. *Journal of Chemical Physics*, **2009**, 131, 124706	3.9	23
135	Relaxation of chlorine anions solvated in small water clusters upon electron photodetachment.: The three lowest potential energy surfaces of the neutral Cl??H2O complex. *Chemical Physics Letters*, **1998**, 293, 309-316	2.5	23
134	A sodium atom in a large water cluster: electron delocalization and infrared spectra. *Journal of Chemical Physics*, **2008**, 128, 154306	3.9	23
133	Segregation of inorganic ions at surfaces of polar nonaqueous liquids. *ChemPhysChem*, **2007**, 8, 1457-63	3.2	23
132	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
131	Small doped 3He clusters: A systematic quantum chemistry approach to fermionic nuclear wave functions and energies. *Journal of Chemical Physics*, **2001**, 115, 10214	3.9	22
130	Quantum dynamics of many-atom systems by the classically based separable potential (CSP) method: Calculations for I(Ar)12 in full dimensionality. *Journal of Chemical Physics*, **1995**, 102, 8855-8864	3.9	22
129	Quantum molecular dynamics of large systems beyond separable approximation: The configuration interaction classical separable potential method. *Journal of Chemical Physics*, **1997**, 107, 8963-8974	3.9	21
128	Photodissociation of hydrogen iodide on the surface of large argon clusters: the orientation of the librational wave function and the scattering from the cluster cage. *Journal of Chemical Physics*, **2004**, 120, 4498-511	3.9	21
127	Ultrafast far-infrared dynamics probed by terahertz pulses: a frequency-domain approach. II. Applications. *Journal of Chemical Physics*, **2005**, 122, 104504	3.9	21
126	Ultrafast far-infrared dynamics probed by terahertz pulses: a frequency domain approach. I. Model systems. *Journal of Chemical Physics*, **2005**, 122, 104503	3.9	21
125	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

124	Increased Binding of Calcium Ions at Positively Curved Phospholipid Membranes. *Journal of Physical Chemistry Letters*, **2017**, 8, 518-523	6.4	20
123	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
122	Microhydration of the magnesium(II) acetate cation in the gas phase. *Journal of Physical Chemistry A*, **2011**, 115, 6813-9	2.8	20
121	Reply to comments on Frontiers Article Behavior of hydroxide at the water/vapor interface *Chemical Physics Letters*, **2009**, 481, 19-21	2.5	20
120	Benchmarking polarizable molecular dynamics simulations of aqueous sodium hydroxide by diffraction measurements. *Journal of Physical Chemistry A*, **2009**, 113, 4022-7	2.8	20
119	Interior and interfacial aqueous solvation of benzene dicarboxylate dianions and their methylated analogues: A combined molecular dynamics and photoelectron spectroscopy study. *Journal of Physical Chemistry A*, **2005**, 109, 5042-9	2.8	20
118	Valence- and dipole-bound anions of the thymine-water complex: ab initio characterization of the potential energy surfaces. *Journal of Physical Chemistry A*, **2006**, 110, 2916-23	2.8	20
117	Effects of End Group Termination on Salting-Out Constants for Triglycine. *Journal of Physical Chemistry Letters*, **2013**, 4, 4069-4073	6.4	19
116	First steps towards dissolution of NaSO4- by water. *Physical Chemistry Chemical Physics*, **2006**, 8, 4294-6	3.6	19
115	Ultrafast Dynamics of Chlorine Water and Bromine Water Radical Complexes Following Electron Photodetachment in Their Anionic Precursors. *Journal of Physical Chemistry A*, **2000**, 104, 6523-6531	2.8	19
114	Anomalous Protein-Protein Interactions in Multivalent Salt Solution. *Journal of Physical Chemistry B*, **2017**, 121, 3000-3006	3.4	18
113	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
112	Guanidinium Pairing Facilitates Membrane Translocation. *Journal of Physical Chemistry B*, **2016**, 120, 143-53	3.4	18
111	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
110	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
109	Characterization of the triple ion [(CH3)4N+ PF6- (CH3)4N+] in the gas-phase. *Chemical Physics Letters*, **2010**, 490, 14-18	2.5	18
108	Cyclobutadiene radical cation. An ab initio study of the Jahn-Teller surface. *Chemical Physics Letters*, **1995**, 234, 395-404	2.5	18
107	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

106	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
105	The C4H4 Potential Energy Surface. 2. The Jahn Teller Stabilization of Ionized Tetrahedrane and Its Rearrangement to Cyclobutadiene Radical Cation. 1. *Journal of Physical Chemistry A*, **1997**, 101, 3918-3924	2.8	17
104	Existence of oriented ion-hydroxide clusters in concentrated aqueous NaCl solution at pH 13. *Journal of Physical Chemistry B*, **2008**, 112, 1262-6	3.4	17
103	Microsolvation of the dicyanamide anion: [N(CN)(2)(-)](H(2)O)n (n = 0-12). *Journal of Physical Chemistry A*, **2007**, 111, 7719-25	2.8	17
102	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
101	From a localized H3O radical to a delocalized H3O+ e- solvent-separated pair by sequential hydration. *Physical Chemistry Chemical Physics*, **2011**, 13, 14003-9	3.6	16
100	Librational Control of Photochemical Reactions in Small Clusters. *Journal of Physical Chemistry A*, **1998**, 102, 7241-7244	2.8	16
99	Binding of divalent cations to acetate: molecular simulations guided by Raman spectroscopy. *Physical Chemistry Chemical Physics*, **2020**, 22, 24014-24027	3.6	16
98	Photodissociation of HBr in and on Arn clusters: the role of the position of the molecule. *Physical Chemistry Chemical Physics*, **2003**, 5, 3394-3401	3.6	15
97	Vibrational line shifts of hydrogen halides in a rare gas environment: HF/DF and HC1/DC1 in Ar matrices and clusters. *Chemical Physics Letters*, **1996**, 259, 62-68	2.5	15
96	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
95	Peptide salt bridge stability: from gas phase via microhydration to bulk water simulations. *Journal of Chemical Physics*, **2012**, 137, 185101	3.9	14
94	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
93	Methylated uracil dimers: potential energy and free energy surfaces. *Physical Chemistry Chemical Physics*, **2000**, 2, 2419-2424	3.6	14
92	Modelization of the protonation of ferrocene using an effective potential parametrized from local-spin density and Hartree Fock calculations. *Chemical Physics Letters*, **1992**, 190, 29-35	2.5	14
91	Nonadiabatic interactions between the ground and low-lying excited electronic states: Vibronic states of the Cl HCl complex. *Journal of Chemical Physics*, **2001**, 115, 5974-5983	3.9	13
90	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
89	Simulation of Raman and Raman optical activity of saccharides in solution. *Physical Chemistry Chemical Physics*, **2020**, 22, 1983-1993	3.6	12

88	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
87	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
86	Membrane Binding of Recoverin: From Mechanistic Understanding to Biological Functionality. *ACS Central Science*, **2017**, 3, 868-874	16.8	12
85	Counterion condensation in short cationic peptides: limiting mobilities beyond the Onsager-Fuoss theory. *Electrophoresis*, **2012**, 33, 981-9	3.6	12
84	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
83	Electrons weakly bound to hydrogen bonded clusters: A pseudopotential model including dispersion interactions. *Journal of Chemical Physics*, **2002**, 117, 5113-5123	3.9	12
82	The Jahn□Teller potential energy surface of H+4. *Chemical Physics Letters*, **1992**, 195, 371-376	2.5	12
81	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
80	Calcium Sensing by Recoverin: Effect of Protein Conformation on Ion Affinity. *Journal of Physical Chemistry Letters*, **2018**, 9, 1613-1619	6.4	11
79	Changes in the hydration structure of imidazole upon protonation: Neutron scattering and molecular simulations. *Journal of Chemical Physics*, **2017**, 146, 185102	3.9	11
78	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
77	Quantum Dynamics and Spectroscopy of Electron Photodetachment in Cl-□H2O and Cl-□D2O Complexes. *Journal of Physical Chemistry A*, **2002**, 106, 12229-12241	2.8	11
76	Potential energy curves for the ground and low-lying excited states of IBr calculated with relativistic effective core potentials and spin□orbit interactions. *Chemical Physics Letters*, **2000**, 321, 281-286	2.5	11
75	Optimal coordinates for separable approximations in quantum dynamics of polyatomic systems: Coordinate choice criteria and error estimates. *Journal of Chemical Physics*, **1999**, 110, 9833-9841	3.9	11
74	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
73	Anomalous surface behavior of hydrated guanidinium ions due to ion pairing. *Journal of Chemical Physics*, **2018**, 148, 144508	3.9	10
72	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
71	The entropy driven hydrophobic effect as a function of solute□solvent interactions. A molecular dynamics study. *Chemical Physics Letters*, **1994**, 217, 319-324	2.5	10

70	Theory of excitation energy transfer in the primary processes of photosynthesis. II. Group symmetry analysis of the bacterial light-harvesting complex. *Chemical Physics*, **1989**, 137, 93-98	2.3	10
69	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
68	Vibrationally resolved spectra from short-time quantum molecular dynamics by the filter-diagonalization method. *Chemical Physics Letters*, **1997**, 280, 177-184	2.5	9
67	Electron photodetachment in C60⁻Quantum molecular dynamics with a non-empirical, 'on-the-fly' calculated potential. *Chemical Physics Letters*, **2000**, 317, 529-534	2.5	9
66	Association and dissociation of nonpolar and polar van der Waals pairs in water. Manifestation of the hydrophobic and hydrophilic effect. *The Journal of Physical Chemistry*, **1994**, 98, 1328-1332		9
65	Quantum dynamics following electron photodetachment in the Ift-Ar2 complex. How good are the new separable and non-separable simulation methods?. *Chemical Physics Letters*, **1997**, 275, 127-136	2.5	8
64	Counter-Ion Effects and Interfacial Properties of Aqueous Tetrabutylammonium Halide Solutions. *Australian Journal of Chemistry*, **2004**, 57, 1211	1.2	8
63	Calculation of the photodetachment cross sections of the HCN- and HNC- dipole-bound anions as described by a one-electron Drude model. *Journal of Chemical Physics*, **2004**, 121, 1824-9	3.9	8
62	Nonadiabatic chemical reaction triggered by electron photodetachment: an ab initio quantum dynamical study. *Physical Review Letters*, **2004**, 93, 048301	7.4	8
61	Sweet taste of heavy water. *Communications Biology*, **2021**, 4, 440	6.7	8
60	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
59	Exploring Fluorescent Dyes at Biomimetic Interfaces with Second Harmonic Generation and Molecular Dynamics. *Langmuir*, **2017**, 33, 3373-3383	4	7
58	Electrophoretic mobilities of neutral analytes and electroosmotic flow markers in aqueous solutions of Hofmeister salts. *Electrophoresis*, **2014**, 35, 617-24	3.6	7
57	Behavior of β-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
56	Librational control of reactions in large clusters. *Chemical Physics Letters*, **1998**, 289, 324-328	2.5	7
55	Aqueous ionic and complementary zwitterionic soluble surfactants: molecular dynamics simulations and sum frequency generation spectroscopy of the surfaces. *Langmuir*, **2006**, 22, 2498-505	4	7
54	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
53	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

52	Embedded Cluster Models for Reactivity of the Hydrated Electron. *Zeitschrift Fur Physikalische Chemie*, **2013**, 227,	3.1	6
51	Specific potassium ion interactions facilitate homocysteine binding to betaine-homocysteine S-methyltransferase. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 2552-64	4.2	6
50	Reactivity of a sodium atom in vibrationally excited water clusters: An ab initio molecular dynamics study. *Chemical Physics Letters*, **2008**, 460, 112-115	2.5	6
49	Optical pump-terahertz probe spectroscopy of dyes in solutions: probing the dynamics of liquid solvent or solid precipitate?. *Journal of Chemical Physics*, **2004**, 120, 912-7	3.9	6
48	Modelling spontaneous chiral stereoselection: the Frank mechanism with racemization. *Journal of the Chemical Society, Faraday Transactions*, **1992**, 88, 1123-1127		6
47	Tail-Oxidized Cholesterol Enhances Membrane Permeability for Small Solutes. *Langmuir*, **2020**, 36, 10438−10447		6
46	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
45	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
44	Interactions of molecular ions with model phospholipid membranes. *Collection of Czechoslovak Chemical Communications*, **2011**, 76, 695-711		5
43	Photoionization of atmospheric gases studied by time-resolved terahertz spectroscopy. *Chemical Physics Letters*, **2008**, 465, 20-24	2.5	5
42	Surface tension from molecular dynamics simulation: Adsorption at the gas-liquid interface. *Israel Journal of Chemistry*, **2003**, 43, 393-397	3.4	5
41	First electronically excited state of the water□argon complex: an analytical fit to the CASPT2 potential. *Chemical Physics Letters*, **1999**, 300, 561-568	2.5	5
40	Oxidation of Cholesterol Changes the Permeability of Lipid Membranes. *Biophysical Journal*, **2017**, 112, 377a	2.9	4
39	A comment on "pH and the surface tension of water" (J. K. Beattie, A. M. Djerdjev, A. Gray-Weale, N. Kallay, J. L□zenkirchen, T. Preo□nin, A. Selmani, J. Colloid Interface Sci. 422 (2014) 54.). *Journal of Colloid and Interface Science*, **2015**, 448, 593	9.3	4
38	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
37	Quantum dynamics of large polyatomic systems using classical separable potentials. *Computers & Chemistry*, **1997**, 21, 419-429		4
36	Chemical oscillations based on photoautocatalysis of ozone. *Chemical Physics Letters*, **2001**, 342, 287-292	2.5	4
35	Double tunneling: An overlooked quantum effect in anionic molecular clusters. *Physical Review Letters*, **2000**, 84, 1140-3	7.4	4

34	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
33	The glycine arginine-rich domain of the RNA-binding protein nucleolin regulates its subcellular localization. *EMBO Journal*, **2021**, 40, e107158	13	4
32	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
31	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
30	Correction to "Unraveling the Complex Nature of the Hydrated Electron". *Journal of Physical Chemistry Letters*, **2013**, 4, 603	6.4	3
29	Is the water-induced potential of mean torsion of n-butane transferable to longer n-alkanes?. *Chemical Physics Letters*, **1993**, 212, 211-217	2.5	3
28	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
27	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
26	Distributions of therapeutically promising neurosteroids in cellular membranes. *Chemistry and Physics of Lipids*, **2017**, 203, 78-86	3.7	2
25	QUANTUM MOLECULAR DYNAMICS SIMULATIONS OF PROCESSES IN LARGE CLUSTERS: METHODS AND APPLICATIONS **1998**, 238-265		2
24	Stability of Charge-Transfer Complexes of CS2 with PH3 and its derivatives: Ab initio MRSDCI/CASSCF Study. *Helvetica Chimica Acta*, **1994**, 77, 1810-1816	2	2
23	The Onset of Ion Solvation by ab initio Calculations: Comparison of Water and Methanol. *Collection of Czechoslovak Chemical Communications*, **2008**, 73, 733-744		2
22	Obtaining 3D Atomistic Structure of Saccharides from Raman/ROA/NMR Spectroscopic Techniques. *Biophysical Journal*, **2020**, 118, 298a	2.9	2
21	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
20	Spectroscopic evidence for a gold-coloured metallic water solution. *Nature*, **2021**, 595, 673-676	50.4	2
19	The Periodic Table. *Journal of Physical Chemistry A*, **2019**, 123, 5837-5848	2.8	1
18	The JPC Periodic Table. *Journal of Physical Chemistry C*, **2019**, 123, 17063-17074	3.8	1
17	The JPC Periodic Table. *Journal of Physical Chemistry Letters*, **2019**, 10, 4051-4062	6.4	1

16	Charges at Aqueous Interfaces: Development of Computational Approaches in Direct Contact with Experiment. *Advances in Chemical Physics*, **2014**, 69-96		1
15	Czech bibliometric system fosters mediocre research. *Nature*, **2009**, 460, 1079	50.4	1
14	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
13	Quantum simulations of vibrational dephasing of molecules in a cryogenic environment: HArF in an argon cluster. *Israel Journal of Chemistry*, **2002**, 42, 157-162	3.4	1
12	Electronic structure of the solvated benzene radical anion.. *Journal of Chemical Physics*, **2022**, 156, 014501	3.9	1
11	Van der Waals Attraction and Coalescence of Aqueous Salt Nanodroplets. *Collection of Czechoslovak Chemical Communications*, **2003**, 68, 2283-2291		1
10	Anisotropic diffusion of membrane proteins at experimental timescales. *Journal of Chemical Physics* , **2021**, 155, 015102	3.9	1
9	Tributes to Victoria Buch. *Journal of Physical Chemistry A*, **2011**, 115, 5709-14	2.8	
8	A chemist realizes that popularity is no measure of strength. *Nature*, **2009**, 460, 555	50.4	
7	Ion Binding to Biomolecules **2009**, 217-230		
6	Photodissociation of Hydrogen Halides in a Cryogenic Rare Gas Environment: A Complex Approach to Simulations of Cluster Experiments **2004**, 467-494		
5	Exact Solution of the Schr□dinger Equation for the Infinite Linear Chain with a Single Trap. *Physica Status Solidi (B): Basic Research*, **1988**, 147, K149-K152	1.3	
4	Physical Properties and Atmospheric Reactivity of Aqueous Sea Salt Micro-Aerosols. *Springer Series in Cluster Physics*, **2003**, 277-293		
3	New Methods in Quantum Molecular Dynamics of Large Polyatomic Systems. *Lecture Notes in Computational Science and Engineering*, **1999**, 365-379	0.3	
2	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	
1	A Non-Exploding Alkali Metal Drop on Water: From Blue Solvated Electrons to Bursting Molten Hydroxide. *Angewandte Chemie*, **2016**, 128, 13213-13216	3.6	