

# Peter J Rossky

## List of Publications by Year in Descending Order

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

97  
papers

9,459  
citations

46  
h-index

97  
g-index

102  
ext. papers

9,895  
ext. citations

9.1  
avg, IF

6.01  
L-index

#	Paper	IF	Citations
97	Single-Molecule Dynamics Reflect IgG Conformational Changes Associated with Ion-Exchange Chromatography. <i>Analytical Chemistry</i> , <b>2021</b> , 93, 11200-11207	7.8	1
96	Machine-Learned Decision Trees for Predicting Gold Nanorod Sizes from Spectra. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 19353-19361	3.8	4
95	Predicting optical spectra for optoelectronic polymers using coarse-grained models and recurrent neural networks. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2020</b> , 117, 13945-13948	11.5	12
94	Direct observation of backbone planarization via side-chain alignment in single bulky-substituted polythiophenes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2018</b> , 115, 2699-2704	11.5	31
93	Fluorescent Proteins Detect Host Structural Rearrangements via Electrostatic Mechanism. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 1203-1206	16.4	7
92	Isotope effects in aqueous solvation of simple halides. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 102306	3.9	6
91	Isotopic equilibria in aqueous clusters at low temperatures: Insights from the MB-pol many-body potential. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 084303	3.9	6
90	Electronic Excited State Lifetimes of Anionic Water Clusters: Dependence on Charge Solvation Motif. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 2304-2309	6.4	14
89	Impact of backbone fluorination on nanoscale morphology and excitonic coupling in polythiophenes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2017</b> , 114, 5113-5118	11.5	36
88	Relating Chromophoric and Structural Disorder in Conjugated Polymers. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 1752-1756	6.4	27
87	Chemical Understanding of the Mechanisms Involved in Mitigation of Charged Impurity Effects by Polar Molecules on Graphene. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 12909-12916	3.8	5
86	Communication: Isotopic effects on tunneling motions in the water trimer. <i>Journal of Chemical Physics</i> , <b>2016</b> , 144, 061101	3.9	11
85	An insight into non-emissive excited states in conjugated polymers. <i>Nature Communications</i> , <b>2015</b> , 6, 8246	17.4	34
84	Resonance Raman Spectroscopy of the T1 Triplet Excited State of Oligothiophenes. <i>Journal of Physical Chemistry Letters</i> , <b>2015</b> , 6, 3521-7	6.4	16
83	Application of a new ensemble conserving quantum dynamics simulation algorithm to liquid para-hydrogen and ortho-deuterium. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 244113	3.9	20
82	A new class of ensemble conserving algorithms for approximate quantum dynamics: Theoretical formulation and model problems. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 244112	3.9	22
81	Isotopic Preferential Solvation of I(-) in Low-Temperature Water Nanoclusters. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 11783-90	3.4	8

80	Surface Isotope Segregation as a Probe of Temperature in Water Nanoclusters. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 2375-9	6.4	11
79	Hot charge-transfer excitons set the time limit for charge separation at donor/acceptor interfaces in organic photovoltaics. <i>Nature Materials</i> , <b>2013</b> , 12, 66-73	27	522
78	Theoretical studies of spectroscopy and dynamics of hydrated electrons. <i>Chemical Reviews</i> , <b>2012</b> , 112, 5641-74	68.1	135
77	Evaporation Length Scales of Confined Water and Some Common Organic Liquids. <i>Journal of Physical Chemistry Letters</i> , <b>2011</b> , 2, 1000-1003	6.4	45
76	Retrospective. Paul F. Barbara (1953-2010). <i>Science</i> , <b>2010</b> , 330, 1191	33.3	1
75	Exploring nanoscale hydrophobic hydration. <i>Faraday Discussions</i> , <b>2010</b> , 146, 13-8; discussion 79-101, 395-401	34.1	33
74	Response of observables for cold anionic water clusters to cluster thermal history. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 2331-7	2.8	32
73	Response to Comment on An electron-water pseudopotential for condensed phase simulation [J. Chem. Phys. 131, 037101 (2009)]. <i>Journal of Chemical Physics</i> , <b>2009</b> , 131, 037102	3.9	15
72	Interior- and surface-bound excess electron states in large water cluster anions. <i>Journal of Chemical Physics</i> , <b>2009</b> , 130, 124319	3.9	45
71	Molecular modeling and simulation of conjugated polymer oligomers: ground and excited state chain dynamics of PPV in the gas phase. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 4983-93	3.4	35
70	Protein denaturation by urea: slash and bond. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2008</b> , 105, 16825-6	11.5	97
69	Nuclear quantum effects on the nonadiabatic decay mechanism of an excited hydrated electron. <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 174508	3.9	26
68	Quantum density fluctuations in liquid neon from linearized path-integral calculations. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	27
67	Quantized time correlation function approach to nonadiabatic decay rates in condensed phase: application to solvated electrons in water and methanol. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 64501	3.9	34
66	Feynman-Kleinert Linearized Path Integral (FK-LPI) Algorithms for Quantum Molecular Dynamics, with Application to Water and He(4). <i>Journal of Chemical Theory and Computation</i> , <b>2006</b> , 2, 1482-91	6.4	45
65	Role of water in electron-initiated processes and radical chemistry: issues and scientific advances. <i>Chemical Reviews</i> , <b>2005</b> , 105, 355-90	68.1	469
64	Characterization of excess electrons in water-cluster anions by quantum simulations. <i>Science</i> , <b>2005</b> , 309, 914-7	33.3	201
63	Quantum Diffusion in Liquid Para-hydrogen: An Application of the Feynman-Kleinert Linearized Path Integral Approximation. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 19799-19808	3.4	68

62	A Theoretical Investigation of the Shape and Hydration Properties of Aqueous Urea: Evidence for Nonplanar Urea Geometry. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 17583-17590	3.4	42
61	Practical evaluation of condensed phase quantum correlation functions: A Feynman-Kleinert variational linearized path integral method. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 12179-12193	3.9	200
60	Stubby Surfactants for Stabilization of Water and CO <sub>2</sub> Emulsions: Trisiloxanes. <i>Langmuir</i> , <b>2003</b> , 19, 3114-3120	4.3	53
59	A second-order Kubo response theory-centroid approach to vibrational energy relaxation for single-mode excitations. <i>Journal of Chemical Physics</i> , <b>2002</b> , 117, 11277-11283	3.9	3
58	Instantaneous normal mode analysis of hydrated electron solvation dynamics. <i>Journal of Chemical Physics</i> , <b>2001</b> , 114, 3598-3611	3.9	37
57	Path integral centroid molecular-dynamics evaluation of vibrational energy relaxation in condensed phase. <i>Journal of Chemical Physics</i> , <b>2001</b> , 115, 8024-8031	3.9	28
56	An ansatz-based variational path integral centroid approach to vibrational energy relaxation in simple liquids. <i>Journal of Chemical Physics</i> , <b>2001</b> , 115, 8014-8023	3.9	20
55	Structural and Electronic Characterization of Chemical and Conformational Defects in Conjugated Polymers. <i>Journal of Physical Chemistry B</i> , <b>2001</b> , 105, 6103-6107	3.4	70
54	Collapse of stiff conjugated polymers with chemical defects into ordered, cylindrical conformations. <i>Nature</i> , <b>2000</b> , 405, 1030-3	50.4	400
53	Perspective on Correlations in the motion of atoms in liquid argon. <i>Theoretical Chemistry Accounts</i> , <b>2000</b> , 103, 263-264	1.9	1
52	Solvent and Intramolecular Effects on the Absorption Spectrum of Betaine-30. <i>Journal of Physical Chemistry A</i> , <b>2000</b> , 104, 899-907	2.8	55
51	The effect of vicinal polar and charged groups on hydrophobic hydration. <i>Biopolymers</i> , <b>1999</b> , 50, 742-50	2.2	29
50	Computer Simulation of the Excited State Dynamics of Betaine-30 in Acetonitrile. <i>Journal of Physical Chemistry A</i> , <b>1999</b> , 103, 9432-9447	2.8	56
49	Nonadiabatic molecular dynamics simulation of photoexcitation experiments for the solvated electron in methanol. <i>Journal of Chemical Physics</i> , <b>1999</b> , 110, 10953-10962	3.9	33
48	Evaluation of Functional Group Contributions to Excess Volumetric Properties of Solvated Molecules. <i>Journal of Physical Chemistry B</i> , <b>1999</b> , 103, 1982-1990	3.4	31
47	Surface topography dependence of biomolecular hydrophobic hydration. <i>Nature</i> , <b>1998</b> , 392, 696-9	50.4	356
46	From Molecules to Materials: Current Trends and Future Directions. <i>Advanced Materials</i> , <b>1998</b> , 10, 1297-1336	13.3	390
45	Non-adiabatic quantum dynamics simulation using classical baths <b>1998</b> ,		6

44	Solvation dynamics of an excess electron in methanol and water. <i>Journal of Chemical Physics</i> , <b>1998</b> , 109, 6390-6395	3.9	43
43	From Molecules to Materials: Current Trends and Future Directions <b>1998</b> , 10, 1297		1
42	From Molecules to Materials: Current Trends and Future Directions <b>1998</b> , 10, 1297		9
41	Mean-field molecular dynamics with surface hopping. <i>Journal of Chemical Physics</i> , <b>1997</b> , 107, 825-834	3.9	286
40	Equilibrium structure, fluctuations, and spectroscopy of a solvated electron in methanol. <i>Journal of Chemical Physics</i> , <b>1997</b> , 107, 1970-1980	3.9	52
39	Evaluation of quantum transition rates from quantum-classical molecular dynamics simulations. <i>Journal of Chemical Physics</i> , <b>1997</b> , 107, 5863-5878	3.9	256
38	Decoherent histories and nonadiabatic quantum molecular dynamics simulations. <i>Journal of Chemical Physics</i> , <b>1997</b> , 107, 8611-8618	3.9	75
37	Size Dependence of Transfer Free Energies. 2. Hard Sphere Models. <i>The Journal of Physical Chemistry</i> , <b>1996</b> , 100, 14166-14177		26
36	Solvent Mode Participation in the Nonradiative Relaxation of the Hydrated Electron. <i>The Journal of Physical Chemistry</i> , <b>1996</b> , 100, 17094-17102		81
35	Quantum decoherence and the isotope effect in condensed phase nonadiabatic molecular dynamics simulations. <i>Journal of Chemical Physics</i> , <b>1996</b> , 104, 5942-5955	3.9	299
34	Electronic and Solvent Relaxation Dynamics of a Photoexcited Aqueous Halide. <i>The Journal of Physical Chemistry</i> , <b>1996</b> , 100, 1295-1302		90
33	The isotope effect in solvation dynamics and nonadiabatic relaxation: A quantum simulation study of the photoexcited solvated electron in D <sub>2</sub> O. <i>Journal of Chemical Physics</i> , <b>1996</b> , 105, 6997-7010	3.9	73
32	Quantum dynamics simulation with approximate eigenstates. <i>Journal of Chemical Physics</i> , <b>1995</b> , 103, 6665-6676	3.9	10
31	Quantum decoherence in mixed quantum-classical systems: Nonadiabatic processes. <i>Journal of Chemical Physics</i> , <b>1995</b> , 103, 8130-8143	3.9	306
30	Simulation and Spectroscopy of Solvation in Water from Ambient to Supercritical Conditions. <i>ACS Symposium Series</i> , <b>1995</b> , 77-92	0.4	7
29	Aqueous solvation dynamics with a quantum mechanical Solute: Computer simulation studies of the photoexcited hydrated electron. <i>Journal of Chemical Physics</i> , <b>1994</b> , 101, 6902-6916	3.9	184
28	Pump-probe spectroscopy of the hydrated electron: A quantum molecular dynamics simulation. <i>Journal of Chemical Physics</i> , <b>1994</b> , 101, 6917-6926	3.9	119
27	Dynamics of chemical processes in polar solvents. <i>Nature</i> , <b>1994</b> , 370, 263-9	50.4	180

26	A comparison of the structure and dynamics of liquid water at hydrophobic and hydrophilic surfaces—molecular dynamics simulation study. <i>Journal of Chemical Physics</i> , <b>1994</b> , 100, 3334-3345	3.9	504
25	The role of solvent intramolecular modes in excess electron solvation dynamics. <i>Journal of Chemical Physics</i> , <b>1993</b> , 99, 515-522	3.9	71
24	A comparison of classical and quantum analyses of electron localization sites in liquid water. <i>Journal of Chemical Physics</i> , <b>1992</b> , 97, 2055-2060	3.9	21
23	On the correlation between like ion pairs in water. <i>Journal of Chemical Physics</i> , <b>1992</b> , 96, 4046-4047	3.9	64
22	Model dependence of quantum isotope effects in liquid water. <i>Journal of Chemical Physics</i> , <b>1991</b> , 95, 3728-3737	3.9	84
21	Transient photophysical hole-burning spectroscopy of the hydrated electron: A quantum dynamical simulation. <i>Journal of Chemical Physics</i> , <b>1989</b> , 90, 6916-6924	3.9	29
20	A priori calculation of the optical absorption spectrum of the hydrated electron. <i>Physical Review Letters</i> , <b>1988</b> , 60, 456-459	7.4	166
19	An electron-water pseudopotential for condensed phase simulation. <i>Journal of Chemical Physics</i> , <b>1987</b> , 86, 3462-3470	3.9	174
18	Quantum simulation study of the hydrated electron. <i>Journal of Chemical Physics</i> , <b>1987</b> , 86, 3471-3485	3.9	174
17	New Approaches to Solvent-Mediated Molecular Interactions. <i>Israel Journal of Chemistry</i> , <b>1986</b> , 27, 156-162	3.9	6
16	Molecular conformational equilibria in liquids. <i>Journal of Chemical Physics</i> , <b>1986</b> , 84, 1712-1723	3.9	102
15	Solvent molecular dynamics in regions of hydrophobic hydration. <i>Journal of Chemical Physics</i> , <b>1986</b> , 84, 2814-2822	3.9	113
14	Alkali halides in water: Ion-solvent correlations and ion-ion potentials of mean force at infinite dilution. <i>Journal of Chemical Physics</i> , <b>1986</b> , 84, 5836-5844	3.9	480
13	The equilibrium solvation structure for the solvent-separated hydrophobic bond. <i>Journal of Chemical Physics</i> , <b>1985</b> , 83, 797-808	3.9	86
12	A quantum mechanical study of structure in liquid H <sub>2</sub> O and D <sub>2</sub> O. <i>Journal of Chemical Physics</i> , <b>1985</b> , 82, 5164-5177	3.9	262
11	The contribution of intramolecular vibrations to the observed structure of liquid water. <i>Journal of Chemical Physics</i> , <b>1985</b> , 82, 5289-5291	3.9	12
10	A complete integral equation formulation in the interaction site formalism. <i>Molecular Physics</i> , <b>1984</b> , 51, 661-674	1.7	95
9	The interionic potential of mean force in a molecular polar solvent from an extended RISM equation. <i>Journal of Chemical Physics</i> , <b>1983</b> , 78, 4133-4144	3.9	231

8	The contribution of hydrogen bonding to the structure of liquid methanol. <i>Journal of Chemical Physics</i> , <b>1983</b> , 78, 7296-7299	3.9	56
7	Corrections to the HNC equation for associating electrolytes. <i>Journal of Chemical Physics</i> , <b>1983</b> , 79, 1419-1426	3.9	51
6	Inconsistent dielectric behaviour of proposed hamiltonian models for ionic solutions. <i>Molecular Physics</i> , <b>1983</b> , 48, 615-618	1.7	11
5	The coupling of long and short range correlations in ISM liquids. <i>Molecular Physics</i> , <b>1983</b> , 50, 1263-1271	1.7	58
4	Application of an extended RISM equation to dipolar and quadrupolar fluids. <i>Journal of Chemical Physics</i> , <b>1982</b> , 77, 509-520	3.9	272
3	Integral equation predictions of liquid state structure for waterlike intermolecular potentials. <i>Journal of Chemical Physics</i> , <b>1982</b> , 77, 1451-1457	3.9	247
2	A realization of $\beta$ structure in liquid water. <i>Journal of Chemical Physics</i> , <b>1981</b> , 74, 6867-6874	3.9	49
1	Solvation: A Molecular Dynamics Study of a Dipeptide in Water. <i>ACS Symposium Series</i> , <b>1980</b> , 23-42	0.4	6