Peter J Rossky

List of Publications by Citations

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	Hot charge-transfer excitons set the time limit for charge separation at donor/acceptor interfaces in organic photovoltaics. *Nature Materials*, **2013**, 12, 66-73	27	522
96	A comparison of the structure and dynamics of liquid water at hydrophobic and hydrophilic surfaces molecular dynamics simulation study. *Journal of Chemical Physics*, **1994**, 100, 3334-3345	3.9	504
95	Alkali halides in water: Ion solvent correlations and ion ion potentials of mean force at infinite dilution. *Journal of Chemical Physics*, **1986**, 84, 5836-5844	3.9	480
94	Role of water in electron-initiated processes and radical chemistry: issues and scientific advances. *Chemical Reviews*, **2005**, 105, 355-90	68.1	469
93	Collapse of stiff conjugated polymers with chemical defects into ordered, cylindrical conformations. *Nature*, **2000**, 405, 1030-3	50.4	400
92	From Molecules to Materials: Current Trends and Future Directions. *Advanced Materials*, **1998**, 10, 1297-1336	21	390
91	Surface topography dependence of biomolecular hydrophobic hydration. *Nature*, **1998**, 392, 696-9	50.4	356
90	Quantum decoherence in mixed quantum-classical systems: Nonadiabatic processes. *Journal of Chemical Physics*, **1995**, 103, 8130-8143	3.9	306
89	Quantum decoherence and the isotope effect in condensed phase nonadiabatic molecular dynamics simulations. *Journal of Chemical Physics*, **1996**, 104, 5942-5955	3.9	299
88	Mean-field molecular dynamics with surface hopping. *Journal of Chemical Physics*, **1997**, 107, 825-834	3.9	286
87	Application of an extended RISM equation to dipolar and quadrupolar fluids. *Journal of Chemical Physics*, **1982**, 77, 509-520	3.9	272
86	A quantum mechanical study of structure in liquid H2O and D2O. *Journal of Chemical Physics*, **1985**, 82, 5164-5177	3.9	262
85	Evaluation of quantum transition rates from quantum-classical molecular dynamics simulations. *Journal of Chemical Physics*, **1997**, 107, 5863-5878	3.9	256
84	Integral equation predictions of liquid state structure for waterlike intermolecular potentials. *Journal of Chemical Physics*, **1982**, 77, 1451-1457	3.9	247
83	The interionic potential of mean force in a molecular polar solvent from an extended RISM equation. *Journal of Chemical Physics*, **1983**, 78, 4133-4144	3.9	231
82	Characterization of excess electrons in water-cluster anions by quantum simulations. *Science*, **2005**, 309, 914-7	33.3	201
81	Practical evaluation of condensed phase quantum correlation functions: A Feynman Kleinert variational linearized path integral method. *Journal of Chemical Physics*, **2003**, 119, 12179-12193	3.9	200

80	Aqueous solvation dynamics with a quantum mechanical Solute: Computer simulation studies of the photoexcited hydrated electron. *Journal of Chemical Physics*, **1994**, 101, 6902-6916	3.9	184
79	Dynamics of chemical processes in polar solvents. *Nature*, **1994**, 370, 263-9	50.4	180
78	An electron–water pseudopotential for condensed phase simulation. *Journal of Chemical Physics*, **1987**, 86, 3462-3470	3.9	174
77	Quantum simulation study of the hydrated electron. *Journal of Chemical Physics*, **1987**, 86, 3471-3485	3.9	174
76	A priori calculation of the optical absorption spectrum of the hydrated electron. *Physical Review Letters*, **1988**, 60, 456-459	7.4	166
75	Theoretical studies of spectroscopy and dynamics of hydrated electrons. *Chemical Reviews*, **2012**, 112, 5641-74	68.1	135
74	Pump–probe spectroscopy of the hydrated electron: A quantum molecular dynamics simulation. *Journal of Chemical Physics*, **1994**, 101, 6917-6926	3.9	119
73	Solvent molecular dynamics in regions of hydrophobic hydration. *Journal of Chemical Physics*, **1986**, 84, 2814-2822	3.9	113
72	Molecular conformational equilibria in liquids. *Journal of Chemical Physics*, **1986**, 84, 1712-1723	3.9	102
71	Protein denaturation by urea: slash and bond. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 16825-6	11.5	97
70	A complete integral equation formulation in the interaction site formalism. *Molecular Physics*, **1984**, 51, 661-674	1.7	95
69	Electronic and Solvent Relaxation Dynamics of a Photoexcited Aqueous Halide. *The Journal of Physical Chemistry*, **1996**, 100, 1295-1302		90
68	The equilibrium solvation structure for the solvent-separated hydrophobic bond. *Journal of Chemical Physics*, **1985**, 83, 797-808	3.9	86
67	Model dependence of quantum isotope effects in liquid water. *Journal of Chemical Physics*, **1991**, 95, 3728-3737	3.9	84
66	Solvent Mode Participation in the Nonradiative Relaxation of the Hydrated Electron. *The Journal of Physical Chemistry*, **1996**, 100, 17094-17102		81
65	Decoherent histories and nonadiabatic quantum molecular dynamics simulations. *Journal of Chemical Physics*, **1997**, 107, 8611-8618	3.9	75
64	The isotope effect in solvation dynamics and nonadiabatic relaxation: A quantum simulation study of the photoexcited solvated electron in D2O. *Journal of Chemical Physics*, **1996**, 105, 6997-7010	3.9	73
63	The role of solvent intramolecular modes in excess electron solvation dynamics. *Journal of Chemical Physics*, **1993**, 99, 515-522	3.9	71

62	Structural and Electronic Characterization of Chemical and Conformational Defects in Conjugated Polymers. *Journal of Physical Chemistry B*, **2001**, 105, 6103-6107	3.4	70
61	Quantum Diffusion in Liquid Para-hydrogen: An Application of the Feynman Kleinert Linearized Path Integral Approximation. *Journal of Physical Chemistry B*, **2004**, 108, 19799-19808	3.4	68
60	On the correlation between like ion pairs in water. *Journal of Chemical Physics*, **1992**, 96, 4046-4047	3.9	64
59	The coupling of long and short range correlations in ISM liquids. *Molecular Physics*, **1983**, 50, 1263-1271	1.7	58
58	Computer Simulation of the Excited State Dynamics of Betaine-30 in Acetonitrile. *Journal of Physical Chemistry A*, **1999**, 103, 9432-9447	2.8	56
57	The contribution of hydrogen bonding to the structure of liquid methanol. *Journal of Chemical Physics*, **1983**, 78, 7296-7299	3.9	56
56	Solvent and Intramolecular Effects on the Absorption Spectrum of Betaine-30. *Journal of Physical Chemistry A*, **2000**, 104, 899-907	2.8	55
55	Stubby Surfactants for Stabilization of Water and CO2 Emulsions: Trisiloxanes. *Langmuir*, **2003**, 19, 3114-3120	4	53
54	Equilibrium structure, fluctuations, and spectroscopy of a solvated electron in methanol. *Journal of Chemical Physics*, **1997**, 107, 1970-1980	3.9	52
53	Corrections to the HNC equation for associating electrolytes. *Journal of Chemical Physics*, **1983**, 79, 1419-1426	3.9	51
52	A realization of V structure in liquid water. *Journal of Chemical Physics*, **1981**, 74, 6867-6874	3.9	49
51	Evaporation Length Scales of Confined Water and Some Common Organic Liquids. *Journal of Physical Chemistry Letters*, **2011**, 2, 1000-1003	6.4	45
50	Interior- and surface-bound excess electron states in large water cluster anions. *Journal of Chemical Physics*, **2009**, 130, 124319	3.9	45
49	Feynman-Kleinert Linearized Path Integral (FK-LPI) Algorithms for Quantum Molecular Dynamics, with Application to Water and He(4). *Journal of Chemical Theory and Computation*, **2006**, 2, 1482-91	6.4	45
48	Solvation dynamics of an excess electron in methanol and water. *Journal of Chemical Physics*, **1998**, 109, 6390-6395	3.9	43
47	A Theoretical Investigation of the Shape and Hydration Properties of Aqueous Urea: Evidence for Nonplanar Urea Geometry. *Journal of Physical Chemistry B*, **2004**, 108, 17583-17590	3.4	42
46	Instantaneous normal mode analysis of hydrated electron solvation dynamics. *Journal of Chemical Physics*, **2001**, 114, 3598-3611	3.9	37
45	Impact of backbone fluorination on nanoscale morphology and excitonic coupling in polythiophenes. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 5113-5118	11.5	36

44	Molecular modeling and simulation of conjugated polymer oligomers: ground and excited state chain dynamics of PPV in the gas phase. *Journal of Physical Chemistry B*, **2008**, 112, 4983-93	3.4	35
43	An insight into non-emissive excited states in conjugated polymers. *Nature Communications*, **2015**, 6, 8246	17.4	34
42	Quantized time correlation function approach to nonadiabatic decay rates in condensed phase: application to solvated electrons in water and methanol. *Journal of Chemical Physics*, **2006**, 125, 64501	3.9	34
41	Exploring nanoscale hydrophobic hydration. *Faraday Discussions*, **2010**, 146, 13-8; discussion 79-101, 395-401	3.6	33
40	Nonadiabatic molecular dynamics simulation of photoexcitation experiments for the solvated electron in methanol. *Journal of Chemical Physics*, **1999**, 110, 10953-10962	3.9	33
39	Response of observables for cold anionic water clusters to cluster thermal history. *Journal of Physical Chemistry A*, **2010**, 114, 2331-7	2.8	32
38	Direct observation of backbone planarization via side-chain alignment in single bulky-substituted polythiophenes. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 2699-2704	11.5	31
37	Evaluation of Functional Group Contributions to Excess Volumetric Properties of Solvated Molecules. *Journal of Physical Chemistry B*, **1999**, 103, 1982-1990	3.4	31
36	The effect of vicinal polar and charged groups on hydrophobic hydration. *Biopolymers*, **1999**, 50, 742-50	2.2	29
35	Transient photophysical hole-burning spectroscopy of the hydrated electron: A quantum dynamical simulation. *Journal of Chemical Physics*, **1989**, 90, 6916-6924	3.9	29
34	Path integral centroid molecular-dynamics evaluation of vibrational energy relaxation in condensed phase. *Journal of Chemical Physics*, **2001**, 115, 8024-8031	3.9	28
33	Relating Chromophoric and Structural Disorder in Conjugated Polymers. *Journal of Physical Chemistry Letters*, **2017**, 8, 1752-1756	6.4	27
32	Quantum density fluctuations in liquid neon from linearized path-integral calculations. *Physical Review B*, **2007**, 75,	3.3	27
31	Size Dependence of Transfer Free Energies. 2. Hard Sphere Models. *The Journal of Physical Chemistry*, **1996**, 100, 14166-14177		26
30	Nuclear quantum effects on the nonadiabatic decay mechanism of an excited hydrated electron. *Journal of Chemical Physics*, **2007**, 127, 174508	3.9	26
29	A new class of ensemble conserving algorithms for approximate quantum dynamics: Theoretical formulation and model problems. *Journal of Chemical Physics*, **2015**, 142, 244112	3.9	22
28	A comparison of classical and quantum analyses of electron localization sites in liquid water. *Journal of Chemical Physics*, **1992**, 97, 2055-2060	3.9	21
27	Application of a new ensemble conserving quantum dynamics simulation algorithm to liquid para-hydrogen and ortho-deuterium. *Journal of Chemical Physics*, **2015**, 142, 244113	3.9	20

26	An ansatz-based variational path integral centroid approach to vibrational energy relaxation in simple liquids. *Journal of Chemical Physics*, **2001**, 115, 8014-8023	3.9	20
25	Resonance Raman Spectroscopy of the T1 Triplet Excited State of Oligothiophenes. *Journal of Physical Chemistry Letters*, **2015**, 6, 3521-7	6.4	16
24	Response to Comment on An electron-water pseudopotential for condensed phase simulation [J. Chem. Phys. 131, 037101 (2009)]. *Journal of Chemical Physics*, **2009**, 131, 037102	3.9	15
23	Electronic Excited State Lifetimes of Anionic Water Clusters: Dependence on Charge Solvation Motif. *Journal of Physical Chemistry Letters*, **2017**, 8, 2304-2309	6.4	14
22	Predicting optical spectra for optoelectronic polymers using coarse-grained models and recurrent neural networks. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 13945-13948	11.5	12
21	The contribution of intramolecular vibrations to the observed structure of liquid water. *Journal of Chemical Physics*, **1985**, 82, 5289-5291	3.9	12
20	Surface Isotope Segregation as a Probe of Temperature in Water Nanoclusters. *Journal of Physical Chemistry Letters*, **2014**, 5, 2375-9	6.4	11
19	Inconsistent dielectric behaviour of proposed hamiltonian models for ionic solutions. *Molecular Physics*, **1983**, 48, 615-618	1.7	11
18	Communication: Isotopic effects on tunneling motions in the water trimer. *Journal of Chemical Physics*, **2016**, 144, 061101	3.9	11
17	Quantum dynamics simulation with approximate eigenstates. *Journal of Chemical Physics*, **1995**, 103, 6665-6676	3.9	10
16	From Molecules to Materials: Current Trends and Future Directions **1998**, 10, 1297		9
15	Isotopic Preferential Solvation of I(-) in Low-Temperature Water Nanoclusters. *Journal of Physical Chemistry B*, **2015**, 119, 11783-90	3.4	8
14	Fluorescent Proteins Detect Host Structural Rearrangements via Electrostatic Mechanism. *Journal of the American Chemical Society*, **2018**, 140, 1203-1206	16.4	7
13	Simulation and Spectroscopy of Solvation in Water from Ambient to Supercritical Conditions. *ACS Symposium Series*, **1995**, 77-92	0.4	7
12	Isotope effects in aqueous solvation of simple halides. *Journal of Chemical Physics*, **2018**, 148, 102306	3.9	6
11	Non-adiabatic quantum dynamics simulation using classical baths **1998**,		6
10	New Approaches to Solvent-Mediated Molecular Interactions. *Israel Journal of Chemistry*, **1986**, 27, 156-162	3.4	6
9	Solvation: A Molecular Dynamics Study of a Dipeptide in Water. *ACS Symposium Series*, **1980**, 23-42	0.4	6

8	Isotopic equilibria in aqueous clusters at low temperatures: Insights from the MB-pol many-body potential. *Journal of Chemical Physics*, **2018**, 148, 084303	3.9	6
7	Chemical Understanding of the Mechanisms Involved in Mitigation of Charged Impurity Effects by Polar Molecules on Graphene. *Journal of Physical Chemistry C*, **2016**, 120, 12909-12916	3.8	5
6	Machine-Learned Decision Trees for Predicting Gold Nanorod Sizes from Spectra. *Journal of Physical Chemistry C*, **2021**, 125, 19353-19361	3.8	4
5	A second-order Kubo response theory-centroid approach to vibrational energy relaxation for single-mode excitations. *Journal of Chemical Physics*, **2002**, 117, 11277-11283	3.9	3
4	Retrospective. Paul F. Barbara (1953-2010). *Science*, **2010**, 330, 1191	33.3	1
3	Perspective on Correlations in the motion of atoms in liquid argon *Theoretical Chemistry Accounts*, **2000**, 103, 263-264	1.9	1
2	Single-Molecule Dynamics Reflect IgG Conformational Changes Associated with Ion-Exchange Chromatography. *Analytical Chemistry*, **2021**, 93, 11200-11207	7.8	1
1	From Molecules to Materials: Current Trends and Future Directions **1998**, 10, 1297		1