Peter J Rossky

List of Publications by Year
in descending order

101 papers	10,422 citations	46918 47 h-index	38300 95 g-index
102 all docs	102 docs citations	102 times ranked	7295 citing authors

#	Article	IF	Citations
1	Hot charge-transfer excitons set the time limit for charge separation at donor/acceptor interfaces in organic photovoltaics. Nature Materials, 2013, 12, 66-73.	13.3	590
2	Role of Water in Electron-Initiated Processes and Radical Chemistry:â€‰ Issues and Scientific Advances. Chemical Reviews, 2005, 105, 355-390.	23.0	560
3	A comparison of the structure and dynamics of liquid water at hydrophobic and hydrophilic surfacesâ€”a molecular dynamics simulation study. Journal of Chemical Physics, 1994, 100, 3334-3345.	1.2	549
4	Alkali halides in water: Ionâ€“solvent correlations and ionâ€“ion potentials of mean force at infinite dilution. Journal of Chemical Physics, 1986, 84, 5836-5844.	1.2	520
5	Collapse of stiff conjugated polymers with chemical defects into ordered, cylindrical conformations. Nature, 2000, 405, 1030-1033.	13.7	433
6	From Molecules to Materials: Current Trends and Future Directions. Advanced Materials, 1998, 10, 1297-1336.	11.1	429
7	Surface topography dependence of biomolecular hydrophobic hydration. Nature, 1998, 392, 696-699.	13.7	378
8	Quantum decoherence in mixed quantumâ€classical systems: Nonadiabatic processes. Journal of Chemical Physics, 1995, 103, 8130-8143.	1.2	350
9	Quantum decoherence and the isotope effect in condensed phase nonadiabatic molecular dynamics simulations. Journal of Chemical Physics, 1996, 104, 5942-5955.	1.2	331
10	Mean-field molecular dynamics with surface hopping. Journal of Chemical Physics, 1997, 107, 825-834.	1.2	306
11	Evaluation of quantum transition rates from quantum-classical molecular dynamics simulations. Journal of Chemical Physics, 1997, 107, 5863-5878.	1.2	299
12	Application of an extended RISM equation to dipolar and quadrupolar fluids. Journal of Chemical Physics, 1982, 77, 509-520.	1.2	290
13	A quantum mechanical study of structure in liquid H2O and D2O. Journal of Chemical Physics, 1985, 82, 5164-5177.	1.2	269
14	Integral equation predictions of liquid state structure for waterlike intermolecular potentials. Journal of Chemical Physics, 1982, 77, 1451-1457.	1.2	268
15	The interionic potential of mean force in a molecular polar solvent from an extended RISM equation. Journal of Chemical Physics, 1983, 78, 4133-4144.	1.2	255
16	Characterization of Excess Electrons in Water-Cluster Anions by Quantum Simulations. Science, 2005, 309, 914-917.	6.0	220
17	Practical evaluation of condensed phase quantum correlation functions: A Feynmanâ€“Kleinert variational linearized path integral method. Journal of Chemical Physics, 2003, 119, 12179-12193.	1.2	217
18	Dynamics of chemical processes in polar solvents. Nature, 1994, 370, 263-269.	13.7	198

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19	Aqueous solvation dynamics with a quantum mechanical Solute: Computer simulation studies of the photoexcited hydrated electron. Journal of Chemical Physics, 1994, 101, 6902-6916.	1.2	196
20	Quantum simulation study of the hydrated electron. Journal of Chemical Physics, 1987, 86, 3471-3485.	1.2	191
21	An electronâ€“water pseudopotential for condensed phase simulation. Journal of Chemical Physics, 1987, 86, 3462-3470.	1.2	186
22	A prioricalculation of the optical absorption spectrum of the hydrated electron. Physical Review Letters, 1988, 60, 456-459.	2.9	173
23	Theoretical Studies of Spectroscopy and Dynamics of Hydrated Electrons. Chemical Reviews, 2012, 112, 5641-5674.	23.0	169
24	Pumpâ€“probe spectroscopy of the hydrated electron: A quantum molecular dynamics simulation. Journal of Chemical Physics, 1994, 101, 6917-6926.	1.2	124
25	Protein denaturation by urea: Slash and bond. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 16825-16826.	3.3	124
26	Solvent molecular dynamics in regions of hydrophobic hydration. Journal of Chemical Physics, 1986, 84, 2814-2822.	1.2	120
27	Molecular conformational equilibria in liquids. Journal of Chemical Physics, 1986, 84, 1712-1723.	1.2	117
28	A complete integral equation formulation in the interaction site formalism. Molecular Physics, 1984, 51, 661-674.	0.8	100
29	Electronic and Solvent Relaxation Dynamics of a Photoexcited Aqueous Halide. The Journal of Physical Chemistry, 1996, 100, 1295-1302.	2.9	96
30	The equilibrium solvation structure for the solventâ€separated hydrophobic bond. Journal of Chemical Physics, 1985, 83, 797-808.	1.2	93
31	Model dependence of quantum isotope effects in liquid water. Journal of Chemical Physics, 1991, 95, 3728-3737.	1.2	92
32	Solvent Mode Participation in the Nonradiative Relaxation of the Hydrated Electron. The Journal of Physical Chemistry, 1996, 100, 17094-17102.	2.9	83
33	Decoherent histories and nonadiabatic quantum molecular dynamics simulations. Journal of Chemical Physics, 1997, 107, 8611-8618.	1.2	81
34	The role of solvent intramolecular modes in excess electron solvation dynamics. Journal of Chemical Physics, 1993, 99, 515-522.	1.2	74
35	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.	1.2	73
36	Structural and Electronic Characterization of Chemical and Conformational Defects in Conjugated Polymers. Journal of Physical Chemistry B, 2001, 105, 6103-6107.	1.2	72

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37	Quantum Diffusion in Liquid Para-hydrogen:Â An Application of the Feynmanâ˜'Kleinert Linearized Path Integral Approximationâ€. Journal of Physical Chemistry B, 2004, 108, 19799-19808.	1.2	70
38	On the correlation between like ion pairs in water. Journal of Chemical Physics, 1992, 96, 4046-4047.	1.2	65
39	Solvent and Intramolecular Effects on the Absorption Spectrum of Betaine-30. Journal of Physical Chemistry A, 2000, 104, 899-907.	1.1	64
40	Computer Simulation of the Excited State Dynamics of Betaine-30 in Acetonitrile. Journal of Physical Chemistry A, 1999, 103, 9432-9447.	1.1	61
41	The contribution of hydrogen bonding to the structure of liquid methanol. Journal of Chemical Physics, 1983, 78, 7296-7299.	1.2	60
42	The coupling of long and short range correlations in ISM liquids. Molecular Physics, 1983, 50, 1263-1271.	0.8	60
43	Stubby Surfactants for Stabilization of Water and CO2Emulsions:Â Trisiloxanes. Langmuir, 2003, 19, 3114-3120.	1.6	59
44	Equilibrium structure, fluctuations, and spectroscopy of a solvated electron in methanol. Journal of Chemical Physics, 1997, 107, 1970-1980.	1.2	55
45	Corrections to the HNC equation for associating electrolytes. Journal of Chemical Physics, 1983, 79, 1419-1426.	1.2	54
46	A realization of â€˜â€˜V structureâ€™â€™ in liquid water. Journal of Chemical Physics, 1981, 74, 6867-6874.	1.2	52
47	Evaporation Length Scales of Confined Water and Some Common Organic Liquids. Journal of Physical Chemistry Letters, 2011, 2, 1000-1003.	2.1	48
48	An insight into non-emissive excited states in conjugated polymers. Nature Communications, 2015, 6, 8246.	5.8	48
49	Feynmanâ˜'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, 1482-1491.	2.3	47
50	Interior- and surface-bound excess electron states in large water cluster anions. Journal of Chemical Physics, 2009, 130, 124319.	1.2	47
51	A Theoretical Investigation of the Shape and Hydration Properties of Aqueous Urea:â€‰ Evidence for Nonplanar Urea Geometry. Journal of Physical Chemistry B, 2004, 108, 17583-17590.	1.2	46
52	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.	3.3	46
53	Solvation dynamics of an excess electron in methanol and water. Journal of Chemical Physics, 1998, 109, 6390-6395.	1.2	45
54	Exploring nanoscale hydrophobic hydration. Faraday Discussions, 2010, 146, 13.	1.6	42

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55	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.	3.3	42
56	Molecular Modeling and Simulation of Conjugated Polymer Oligomers:â€‰ Ground and Excited State Chain Dynamics of PPV in the Gas Phase. Journal of Physical Chemistry B, 2008, 112, 4983-4993.	1.2	39
57	Instantaneous normal mode analysis of hydrated electron solvation dynamics. Journal of Chemical Physics, 2001, 114, 3598-3611.	1.2	38
58	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, 064501.	1.2	36
59	Nonadiabatic molecular dynamics simulation of photoexcitation experiments for the solvated electron in methanol. Journal of Chemical Physics, 1999, 110, 10953-10962.	1.2	35
60	Evaluation of Functional Group Contributions to Excess Volumetric Properties of Solvated Molecules. Journal of Physical Chemistry B, 1999, 103, 1982-1990.	1.2	34
61	Response of Observables for Cold Anionic Water Clusters to Cluster Thermal History. Journal of Physical Chemistry A, 2010, 114, 2331-2337.	1.1	33
62	The effect of vicinal polar and charged groups on hydrophobic hydration. , 1999, 50, 742-750.		32
63	Relating Chromophoric and Structural Disorder in Conjugated Polymers. Journal of Physical Chemistry Letters, 2017, 8, 1752-1756.	2.1	31
64	Transient photophysical holeâ€burning spectroscopy of the hydrated electron: A quantum dynamical simulation. Journal of Chemical Physics, 1989, 90, 6916-6924.	1.2	30
65	Path integral centroid molecular-dynamics evaluation of vibrational energy relaxation in condensed phase. Journal of Chemical Physics, 2001, 115, 8024-8031.	1.2	30
66	Nuclear quantum effects on the nonadiabatic decay mechanism of an excited hydrated electron. Journal of Chemical Physics, 2007, 127, 174508.	1.2	29
67	Quantum density fluctuations in liquid neon from linearized path-integral calculations. Physical Review B, 2007, 75, .	1.1	28
68	Size Dependence of Transfer Free Energies. 2. Hard Sphere Models. The Journal of Physical Chemistry, 1996, 100, 14166-14177.	2.9	27
69	A new class of ensemble conserving algorithms for approximate quantum dynamics: Theoretical formulation and model problems. Journal of Chemical Physics, 2015, 142, 244112.	1.2	26
70	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.	3.3	24
71	Application of a new ensemble conserving quantum dynamics simulation algorithm to liquid para-hydrogen and ortho-deuterium. Journal of Chemical Physics, 2015, 142, 244113.	1.2	22
72	A comparison of classical and quantum analyses of electron localization sites in liquid water. Journal of Chemical Physics, 1992, 97, 2055-2060.	1.2	21

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73	An ansatz-based variational path integral centroid approach to vibrational energy relaxation in simple liquids. Journal of Chemical Physics, 2001, 115, 8014-8023.	1.2	20
74	Communication: Isotopic effects on tunneling motions in the water trimer. Journal of Chemical Physics, 2016, 144, 061101.	1.2	19
75	Resonance Raman Spectroscopy of the T₁ Triplet Excited State of Oligothiophenes. Journal of Physical Chemistry Letters, 2015, 6, 3521-3527.	2.1	16
76	Machine-Learned Decision Trees for Predicting Gold Nanorod Sizes from Spectra. Journal of Physical Chemistry C, 2021, 125, 19353-19361.	1.5	16
77	Response to â€œComment on â€˜An electron-water pseudopotential for condensed phase simulationâ€™â€‰â€•[J. Chem. Phys. 131, 037101 (2009)]. Journal of Chemical Physics, 2009, 131, .	1.2	15
78	Electronic Excited State Lifetimes of Anionic Water Clusters: Dependence on Charge Solvation Motif. Journal of Physical Chemistry Letters, 2017, 8, 2304-2309.	2.1	15
79	The contribution of intramolecular vibrations to the observed structure of liquid water. Journal of Chemical Physics, 1985, 82, 5289-5291.	1.2	12
80	Surface Isotope Segregation as a Probe of Temperature in Water Nanoclusters. Journal of Physical Chemistry Letters, 2014, 5, 2375-2379.	2.1	12
81	Fluorescent Proteins Detect Host Structural Rearrangements via Electrostatic Mechanism. Journal of the American Chemical Society, 2018, 140, 1203-1206.	6.6	12
82	Isotopic equilibria in aqueous clusters at low temperatures: Insights from the MB-pol many-body potential. Journal of Chemical Physics, 2018, 148, 084303.	1.2	12
83	Inconsistent dielectric behaviour of proposed hamiltonian models for ionic solutions. Molecular Physics, 1983, 48, 615-618.	0.8	11
84	Isotopic Preferential Solvation of I^{â€“} in Low-Temperature Water Nanoclusters. Journal of Physical Chemistry B, 2015, 119, 11783-11790.	1.2	11
85	Quantum dynamics simulation with approximate eigenstates. Journal of Chemical Physics, 1995, 103, 6665-6676.	1.2	10
86	From Molecules to Materials: Current Trends and Future Directions. , 1998, 10, 1297.		9
87	Simulation and Spectroscopy of Solvation in Water from Ambient to Supercritical Conditions. ACS Symposium Series, 1995, , 77-92.	0.5	8
88	Solvation: A Molecular Dynamics Study of a Dipeptide in Water. ACS Symposium Series, 1980, , 23-42.	0.5	7
89	Isotope effects in aqueous solvation of simple halides. Journal of Chemical Physics, 2018, 148, 102306.	1.2	7
90	Single-Molecule Dynamics Reflect IgG Conformational Changes Associated with Ion-Exchange Chromatography. Analytical Chemistry, 2021, 93, 11200-11207.	3.2	7

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91	New Approaches to Solventâ€Mediated Molecular Interactions. Israel Journal of Chemistry, 1986, 27, 156-162.	1.0	6
92	Non-adiabatic quantum dynamics simulation using classical baths. , 1998, , .		6
93	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.	1.5	5
94	Molecules at the edge. Nature, 2001, 410, 645-647.	13.7	3
95	A second-order Kubo response theory-centroid approach to vibrational energy relaxation for single-mode excitations. Journal of Chemical Physics, 2002, 117, 11277-11283.	1.2	3
96	Perspective on "Correlations in the motion of atoms in liquid argon". Theoretical Chemistry Accounts, 2000, 103, 263-264.	0.5	1
97	Paul F. Barbara (1953â€“2010). Science, 2010, 330, 1191-1191.	6.0	1
98	From Molecules to Materials: Current Trends and Future Directions. , 1998, 10, 1297.		1
99	Quantum simulation of electronic dynamics in solution. AIP Conference Proceedings, 1994, , .	0.3	0
100	An Autobiographical History of Peter J. Rossky. Journal of Physical Chemistry B, 2020, 124, 10594-10597.	1.2	0
101	The Age of Direct Chemical Dynamics. Accounts of Chemical Research, 2022, 55, 471-472.	7.6	0