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	The Age of Direct Chemical Dynamics. Accounts of Chemical Research, 2022, 55, 471-472.	7.6	0
2	Single-Molecule Dynamics Reflect IgG Conformational Changes Associated with Ion-Exchange Chromatography. Analytical Chemistry, 2021, 93, 11200-11207.	3.2	7
3	Machine-Learned Decision Trees for Predicting Gold Nanorod Sizes from Spectra. Journal of Physical Chemistry C, 2021, 125, 19353-19361.	1.5	16
4	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
5	An Autobiographical History of Peter J. Rossky. Journal of Physical Chemistry B, 2020, 124, 10594-10597.	1.2	0
6	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
7	Fluorescent Proteins Detect Host Structural Rearrangements via Electrostatic Mechanism. Journal of the American Chemical Society, 2018, 140, 1203-1206.	6.6	12
8	Isotope effects in aqueous solvation of simple halides. Journal of Chemical Physics, 2018, 148, 102306.	1.2	7
9	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
10	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
11	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
12	Relating Chromophoric and Structural Disorder in Conjugated Polymers. Journal of Physical Chemistry Letters, 2017, 8, 1752-1756.	2.1	31
13	Communication: Isotopic effects on tunneling motions in the water trimer. Journal of Chemical Physics, 2016, 144, 061101.	1.2	19
14	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
15	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
16	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
17	Isotopic Preferential Solvation of I^{â€“} in Low-Temperature Water Nanoclusters. Journal of Physical Chemistry B, 2015, 119, 11783-11790.	1.2	11
18	An insight into non-emissive excited states in conjugated polymers. Nature Communications, 2015, 6, 8246.	5.8	48

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19	Resonance Raman Spectroscopy of the T₁ Triplet Excited State of Oligothiophenes. Journal of Physical Chemistry Letters, 2015, 6, 3521-3527.	2.1	16
20	Surface Isotope Segregation as a Probe of Temperature in Water Nanoclusters. Journal of Physical Chemistry Letters, 2014, 5, 2375-2379.	2.1	12
21	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
22	Theoretical Studies of Spectroscopy and Dynamics of Hydrated Electrons. Chemical Reviews, 2012, 112, 5641-5674.	23.0	169
23	Evaporation Length Scales of Confined Water and Some Common Organic Liquids. Journal of Physical Chemistry Letters, 2011, 2, 1000-1003.	2.1	48
24	Paul F. Barbara (1953â€“2010). Science, 2010, 330, 1191-1191.	6.0	1
25	Exploring nanoscale hydrophobic hydration. Faraday Discussions, 2010, 146, 13.	1.6	42
26	Response of Observables for Cold Anionic Water Clusters to Cluster Thermal History. Journal of Physical Chemistry A, 2010, 114, 2331-2337.	1.1	33
27	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
28	Interior- and surface-bound excess electron states in large water cluster anions. Journal of Chemical Physics, 2009, 130, 124319.	1.2	47
29	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
30	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
31	Nuclear quantum effects on the nonadiabatic decay mechanism of an excited hydrated electron. Journal of Chemical Physics, 2007, 127, 174508.	1.2	29
32	Quantum density fluctuations in liquid neon from linearized path-integral calculations. Physical Review B, 2007, 75, .	1.1	28
33	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
34	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
35	Characterization of Excess Electrons in Water-Cluster Anions by Quantum Simulations. Science, 2005, 309, 914-917.	6.0	220
36	Role of Water in Electron-Initiated Processes and Radical Chemistry:â€‰ Issues and Scientific Advances. Chemical Reviews, 2005, 105, 355-390.	23.0	560

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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	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
39	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
40	Stubby Surfactants for Stabilization of Water and CO2Emulsions:Â Trisiloxanes. Langmuir, 2003, 19, 3114-3120.	1.6	59
41	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
42	Structural and Electronic Characterization of Chemical and Conformational Defects in Conjugated Polymers. Journal of Physical Chemistry B, 2001, 105, 6103-6107.	1.2	72
43	Molecules at the edge. Nature, 2001, 410, 645-647.	13.7	3
44	Instantaneous normal mode analysis of hydrated electron solvation dynamics. Journal of Chemical Physics, 2001, 114, 3598-3611.	1.2	38
45	Path integral centroid molecular-dynamics evaluation of vibrational energy relaxation in condensed phase. Journal of Chemical Physics, 2001, 115, 8024-8031.	1.2	30
46	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
47	Collapse of stiff conjugated polymers with chemical defects into ordered, cylindrical conformations. Nature, 2000, 405, 1030-1033.	13.7	433
48	Perspective on "Correlations in the motion of atoms in liquid argon". Theoretical Chemistry Accounts, 2000, 103, 263-264.	0.5	1
49	Solvent and Intramolecular Effects on the Absorption Spectrum of Betaine-30. Journal of Physical Chemistry A, 2000, 104, 899-907.	1.1	64
50	The effect of vicinal polar and charged groups on hydrophobic hydration. , 1999, 50, 742-750.		32
51	Computer Simulation of the Excited State Dynamics of Betaine-30 in Acetonitrile. Journal of Physical Chemistry A, 1999, 103, 9432-9447.	1.1	61
52	Nonadiabatic molecular dynamics simulation of photoexcitation experiments for the solvated electron in methanol. Journal of Chemical Physics, 1999, 110, 10953-10962.	1.2	35
53	Evaluation of Functional Group Contributions to Excess Volumetric Properties of Solvated Molecules. Journal of Physical Chemistry B, 1999, 103, 1982-1990.	1.2	34
54	Surface topography dependence of biomolecular hydrophobic hydration. Nature, 1998, 392, 696-699.	13.7	378

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55	From Molecules to Materials: Current Trends and Future Directions. Advanced Materials, 1998, 10, 1297-1336.	11.1	429
56	Non-adiabatic quantum dynamics simulation using classical baths. , 1998, , .		6
57	Solvation dynamics of an excess electron in methanol and water. Journal of Chemical Physics, 1998, 109, 6390-6395.	1.2	45
58	From Molecules to Materials: Current Trends and Future Directions. , 1998, 10, 1297.		1
59	From Molecules to Materials: Current Trends and Future Directions. , 1998, 10, 1297.		9
60	Mean-field molecular dynamics with surface hopping. Journal of Chemical Physics, 1997, 107, 825-834.	1.2	306
61	Equilibrium structure, fluctuations, and spectroscopy of a solvated electron in methanol. Journal of Chemical Physics, 1997, 107, 1970-1980.	1.2	55
62	Evaluation of quantum transition rates from quantum-classical molecular dynamics simulations. Journal of Chemical Physics, 1997, 107, 5863-5878.	1.2	299
63	Decoherent histories and nonadiabatic quantum molecular dynamics simulations. Journal of Chemical Physics, 1997, 107, 8611-8618.	1.2	81
64	Solvent Mode Participation in the Nonradiative Relaxation of the Hydrated Electron. The Journal of Physical Chemistry, 1996, 100, 17094-17102.	2.9	83
65	Quantum decoherence and the isotope effect in condensed phase nonadiabatic molecular dynamics simulations. Journal of Chemical Physics, 1996, 104, 5942-5955.	1.2	331
66	Electronic and Solvent Relaxation Dynamics of a Photoexcited Aqueous Halide. The Journal of Physical Chemistry, 1996, 100, 1295-1302.	2.9	96
67	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
68	Size Dependence of Transfer Free Energies. 2. Hard Sphere Models. The Journal of Physical Chemistry, 1996, 100, 14166-14177.	2.9	27
69	Quantum dynamics simulation with approximate eigenstates. Journal of Chemical Physics, 1995, 103, 6665-6676.	1.2	10
70	Quantum decoherence in mixed quantumâ€classical systems: Nonadiabatic processes. Journal of Chemical Physics, 1995, 103, 8130-8143.	1.2	350
71	Simulation and Spectroscopy of Solvation in Water from Ambient to Supercritical Conditions. ACS Symposium Series, 1995, , 77-92.	0.5	8
72	Quantum simulation of electronic dynamics in solution. AIP Conference Proceedings, 1994, , .	0.3	0

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73	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
74	Pumpâ€“probe spectroscopy of the hydrated electron: A quantum molecular dynamics simulation. Journal of Chemical Physics, 1994, 101, 6917-6926.	1.2	124
75	Dynamics of chemical processes in polar solvents. Nature, 1994, 370, 263-269.	13.7	198
76	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
77	The role of solvent intramolecular modes in excess electron solvation dynamics. Journal of Chemical Physics, 1993, 99, 515-522.	1.2	74
78	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
79	On the correlation between like ion pairs in water. Journal of Chemical Physics, 1992, 96, 4046-4047.	1.2	65
80	Model dependence of quantum isotope effects in liquid water. Journal of Chemical Physics, 1991, 95, 3728-3737.	1.2	92
81	Transient photophysical holeâ€burning spectroscopy of the hydrated electron: A quantum dynamical simulation. Journal of Chemical Physics, 1989, 90, 6916-6924.	1.2	30
82	A prioricalculation of the optical absorption spectrum of the hydrated electron. Physical Review Letters, 1988, 60, 456-459.	2.9	173
83	An electronâ€“water pseudopotential for condensed phase simulation. Journal of Chemical Physics, 1987, 86, 3462-3470.	1.2	186
84	Quantum simulation study of the hydrated electron. Journal of Chemical Physics, 1987, 86, 3471-3485.	1.2	191
85	Solvent molecular dynamics in regions of hydrophobic hydration. Journal of Chemical Physics, 1986, 84, 2814-2822.	1.2	120
86	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
87	New Approaches to Solventâ€Mediated Molecular Interactions. Israel Journal of Chemistry, 1986, 27, 156-162.	1.0	6
88	Molecular conformational equilibria in liquids. Journal of Chemical Physics, 1986, 84, 1712-1723.	1.2	117
89	The equilibrium solvation structure for the solventâ€separated hydrophobic bond. Journal of Chemical Physics, 1985, 83, 797-808.	1.2	93
90	A quantum mechanical study of structure in liquid H2O and D2O. Journal of Chemical Physics, 1985, 82, 5164-5177.	1.2	269

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91	The contribution of intramolecular vibrations to the observed structure of liquid water. Journal of Chemical Physics, 1985, 82, 5289-5291.	1.2	12
92	A complete integral equation formulation in the interaction site formalism. Molecular Physics, 1984, 51, 661-674.	0.8	100
93	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
94	The contribution of hydrogen bonding to the structure of liquid methanol. Journal of Chemical Physics, 1983, 78, 7296-7299.	1.2	60
95	Corrections to the HNC equation for associating electrolytes. Journal of Chemical Physics, 1983, 79, 1419-1426.	1.2	54
96	Inconsistent dielectric behaviour of proposed hamiltonian models for ionic solutions. Molecular Physics, 1983, 48, 615-618.	0.8	11
97	The coupling of long and short range correlations in ISM liquids. Molecular Physics, 1983, 50, 1263-1271.	0.8	60
98	Application of an extended RISM equation to dipolar and quadrupolar fluids. Journal of Chemical Physics, 1982, 77, 509-520.	1.2	290
99	Integral equation predictions of liquid state structure for waterlike intermolecular potentials. Journal of Chemical Physics, 1982, 77, 1451-1457.	1.2	268
100	A realization of â€˜â€˜V structureâ€™â€™ in liquid water. Journal of Chemical Physics, 1981, 74, 6867-6874.	1.2	52
101	Solvation: A Molecular Dynamics Study of a Dipeptide in Water. ACS Symposium Series, 1980, , 23-42.	0.5	7