Benjamin F Schwartz

List of Publications by Year
in descending order

189 papers	12,516 citations	26630 56 h-index	26613 107 g-index
192 all docs	192 docs citations	192 times ranked	10132 citing authors

#	Article	IF	Citations
1	CONJUGATEDPOLYMERS ASMOLECULARMATERIALS: How Chain Conformation and Film Morphology Influence Energy Transfer and Interchain Interactions. Annual Review of Physical Chemistry, 2003, 54, 141-172.	10.8	901
2	Controlling Interchain Interactions in Conjugated Polymers:â€‰ The Effects of Chain Morphology on Excitonâ^'Exciton Annihilation and Aggregation in MEHâ^'PPV Films. Journal of Physical Chemistry B, 2000, 104, 237-255.	2.6	817
3	Conjugated polymer aggregates in solution: Control of interchain interactions. Journal of Chemical Physics, 1999, 110, 4068-4078.	3.0	709
4	Control of Energy Transfer in Oriented Conjugated Polymer-Mesoporous Silica Composites. Science, 2000, 288, 652-656.	12.6	642
5	New Developments in the Photonic Applications of Conjugated Polymers. Accounts of Chemical Research, 1997, 30, 430-436.	15.6	485
6	Quantum decoherence and the isotope effect in condensed phase nonadiabatic molecular dynamics simulations. Journal of Chemical Physics, 1996, 104, 5942-5955.	3.0	331
7	Reappraising the Need for Bulk Heterojunctions in Polymerâ^'Fullerene Photovoltaics: The Role of Carrier Transport in All-Solution-Processed P3HT/PCBM Bilayer Solar Cells. Journal of Physical Chemistry C, 2009, 113, 20050-20060.	3.1	303
8	Laser emission from solutions and films containing semiconducting polymer and titanium dioxide nanocrystals. Chemical Physics Letters, 1996, 256, 424-430.	2.6	295
9	Direct observation of fast proton transfer: femtosecond photophysics of 3-hydroxyflavone. The Journal of Physical Chemistry, 1992, 96, 3591-3598.	2.9	246
10	Does the Hydrated Electron Occupy a Cavity?. Science, 2010, 329, 65-69.	12.6	212
11	Aqueous solvation dynamics with a quantum mechanical Solute: Computer simulation studies of the photoexcited hydrated electron. Journal of Chemical Physics, 1994, 101, 6902-6916.	3.0	196
12	The Effects of Crystallinity on Charge Transport and the Structure of Sequentially Processed F₄TCNQâ€Doped Conjugated Polymer Films. Advanced Functional Materials, 2017, 27, 1702654.	14.9	190
13	Improving the performance of conjugated polymer-based devices by control of interchain interactions and polymer film morphology. Applied Physics Letters, 2000, 76, 2454-2456.	3.3	181
14	Mean-field dynamics with stochastic decoherence (MF-SD): A new algorithm for nonadiabatic mixed quantum/classical molecular-dynamics simulations with nuclear-induced decoherence. Journal of Chemical Physics, 2005, 123, 234106.	3.0	181
15	Overcoming Film Quality Issues for Conjugated Polymers Doped with F₄TCNQ by Solution Sequential Processing: Hall Effect, Structural, and Optical Measurements. Journal of Physical Chemistry Letters, 2015, 6, 4786-4793.	4.6	175
16	Single-shot two-photon exposure of commercial photoresist for the production of three-dimensional structures. Optics Letters, 1998, 23, 1745.	3.3	159
17	Improving the Reproducibility of P3HT:PCBM Solar Cells by Controlling the PCBM/Cathode Interface. Journal of Physical Chemistry C, 2009, 113, 18978-18982.	3.1	150
18	Plastic lasers: Semiconducting polymers as a new class of solid-state laser materials. Synthetic Metals, 1997, 84, 455-462.	3.9	148

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19	Charge-carrier dynamics in hybrid plasmonic organic solar cells with Ag nanoparticles. Applied Physics Letters, 2011, 98, .	3.3	138
20	Ultrafast studies of photochromic spiropyrans in solution. Journal of the American Chemical Society, 1992, 114, 10921-10927.	13.7	136
21	Activation of Snap-Top Capped Mesoporous Silica Nanocontainers Using Two Near-Infrared Photons. Journal of the American Chemical Society, 2013, 135, 14000-14003.	13.7	132
22	Pumpâ€“probe spectroscopy of the hydrated electron: A quantum molecular dynamics simulation. Journal of Chemical Physics, 1994, 101, 6917-6926.	3.0	124
23	Direct femtosecond measurements of single collision dominated geminate recombination times of small molecules in liquids. Chemical Physics Letters, 1993, 203, 503-508.	2.6	123
24	Exciton-exciton annihilation and the production of interchain species in conjugated polymer films:â€ƒComparing the ultrafast stimulated emission and photoluminescence dynamics of MEH-PPV. Physical Review B, 2004, 69, .	3.2	120
25	â€œPlasticâ€•lasers: Comparison of gain narrowing with a soluble semiconducting polymer in waveguides and microcavities. Applied Physics Letters, 1997, 70, 3191-3193.	3.3	112
26	Near-field two-photon nanolithography using an apertureless optical probe. Applied Physics Letters, 2002, 81, 3663-3665.	3.3	108
27	Self-Assembling Fullerenes for Improved Bulk-Heterojunction Photovoltaic Devices. Journal of the American Chemical Society, 2008, 130, 17290-17292.	13.7	107
28	Controlling optical gain in semiconducting polymers with nanoscale chain positioning and alignment. Nature Nanotechnology, 2007, 2, 647-652.	31.5	102
29	Phthalocyanineâ^'Azacrownâ^'Fullerene Multicomponent System:Â Synthesis, Photoinduced Processes, and Electrochemistry#. Organic Letters, 1999, 1, 1807-1810.	4.6	99
30	How Does the Solvent Control Electron Transfer? Experimental and Theoretical Studies of the Simplest Charge Transfer Reaction. Journal of Physical Chemistry B, 2001, 105, 12230-12241.	2.6	98
31	Quantifying field-scale soil moisture using electrical resistivity imaging. Journal of Hydrology, 2008, 362, 234-246.	5.4	96
32	Room to Improve Conjugated Polymer-Based Solar Cells: Understanding How Thermal Annealing Affects the Fullerene Component of a Bulk Heterojunction Photovoltaic Device. Journal of Physical Chemistry C, 2008, 112, 18711-18716.	3.1	94
33	Solution processing of conjugated polymers: the effects of polymer solubility on the morphology and electronic properties of semiconducting polymer films. Journal of Photochemistry and Photobiology A: Chemistry, 2001, 144, 21-30.	3.9	90
34	Dodecaboraneâ€Based Dopants Designed to Shield Anion Electrostatics Lead to Increased Carrier Mobility in a Doped Conjugated Polymer. Advanced Materials, 2019, 31, e1805647.	21.0	90
35	Interchain and intrachain exciton transport in conjugated polymers: ultrafast studies of energy migration in aligned MEH-PPV/mesoporous silica composites. Synthetic Metals, 2001, 116, 35-40.	3.9	87
36	Nonlinear, Nonpolar Solvation Dynamics in Water:Â The Roles of Electrostriction and Solvent Translation in the Breakdown of Linear Response. Journal of Physical Chemistry B, 2000, 104, 5382-5394.	2.6	85

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37	Near-Field Scanning Optical Microscopy (NSOM) Studies of the Relationship between Interchain Interactions, Morphology, Photodamage, and Energy Transport in Conjugated Polymer Films. Journal of Physical Chemistry B, 2001, 105, 5153-5160.	2.6	82
38	Sequential Processing for Organic Photovoltaics: Design Rules for Morphology Control by Tailored Semiâ€Orthogonal Solvent Blends. Advanced Energy Materials, 2015, 5, 1402020.	19.5	82
39	Ultrafast competition between energy and charge transfer in a functionalized electron donor/fullerene derivative. Chemical Physics Letters, 2000, 327, 253-262.	2.6	78
40	Investigation of Spectroscopic Intermediates during Copper-Binding and TPQ Formation in Wild-Type and Active-Site Mutants of a Copper-Containing Amine Oxidase from Yeast. Biochemistry, 2000, 39, 3690-3698.	2.5	74
41	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.	3.0	73
42	Kinetic Analysis of Oxygen Utilization during Cofactor Biogenesis in a Copper-Containing Amine Oxidase from Yeast. Biochemistry, 2000, 39, 3699-3707.	2.5	73
43	The Role of Copper in Topa Quinone Biogenesis and Catalysis, as Probed by Azide Inhibition of a Copper Amine Oxidase from Yeastâ€. Biochemistry, 2001, 40, 2954-2963.	2.5	71
44	Ionomeric control of interchain interactions, morphology, and the electronic properties of conjugated polymer solutions and films. Journal of Chemical Physics, 2002, 116, 8198-8208.	3.0	70
45	Hydrated electrons as a probe of local anisotropy: Simulations of ultrafast polarization-dependent spectral hole burning. Physical Review Letters, 1994, 72, 3282-3285.	7.8	68
46	Ultrafast studies of stimulated emission and gain in solid films of conjugated polymers. Chemical Physics Letters, 1997, 265, 327-333.	2.6	66
47	Linear Response Breakdown in Solvation Dynamics Induced by Atomic Electron-Transfer Reactions. Science, 2008, 321, 1817-1822.	12.6	65
48	Discovery of a Novel 2,6-Disubstituted Glucosamine Series of Potent and Selective Hexokinase 2 Inhibitors. ACS Medicinal Chemistry Letters, 2016, 7, 217-222.	2.8	64
49	Mechanisms of the ultrafast production and recombination of solvated electrons in weakly polar fluids: Comparison of multiphoton ionization and detachment via the charge-transfer-to-solvent transition of Naâ^' in THF. Journal of Chemical Physics, 2000, 113, 11245-11257.	3.0	63
50	Optical Control of Electrons During Electron Transfer. Science, 2001, 293, 462-465.	12.6	63
51	Dopant-Induced Ordering of Amorphous Regions in Regiorandom P3HT. Journal of Physical Chemistry Letters, 2019, 10, 4929-4934.	4.6	63
52	Exploring the Role of Decoherence in Condensed-Phase Nonadiabatic Dynamics:Â A Comparison of Different Mixed Quantum/Classical Simulation Algorithms for the Excited Hydrated Electron. Journal of Physical Chemistry B, 2006, 110, 20055-20066.	2.6	62
53	Conjugated polymers as solid-state laser materials. Synthetic Metals, 1997, 91, 35-40.	3.9	61
54	Hybrid conjugated polymer solar cells using patterned GaAs nanopillars. Applied Physics Letters, 2010, 97, 013107.	3.3	60

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55	Response to Comments on â€œDoes the Hydrated Electron Occupy a Cavity?â€• Science, 2011, 331, 1387-1387.	12.6	58
56	To Be or Not to Be in a Cavity: The Hydrated Electron Dilemma. Journal of Physical Chemistry B, 2013, 117, 14173-14182.	2.6	58
57	The Nature of Interchain Excitations in Conjugated Polymers:â€‰ Spatially-Varying Interfacial Solvatochromism of Annealed MEH-PPV Films Studied by Near-Field Scanning Optical Microscopy (NSOM). Journal of Physical Chemistry B, 2002, 106, 9496-9506.	2.6	57
58	Designing Conjugated Polymers for Molecular Doping: The Roles of Crystallinity, Swelling, and Conductivity in Sequentially-Doped Selenophene-Based Copolymers. Chemistry of Materials, 2019, 31, 73-82.	6.7	56
59	Evaporation vs Solution Sequential Doping of Conjugated Polymers: F₄TCNQ Doping of Micrometer-Thick P3HT Films for Thermoelectrics. Journal of Physical Chemistry C, 2019, 123, 22711-22724.	3.1	55
60	Femtosecond studies of hydrated electron recombination following multiphoton ionization at 390 nm. Chemical Physics Letters, 1994, 231, 504-510.	2.6	54
61	Long-lived photoinduced polaron formation in conjugated polyelectrolyte-fullerene assemblies. Science, 2015, 348, 1340-1343.	12.6	53
62	Tunable Dopants with Intrinsic Counterion Separation Reveal the Effects of Electron Affinity on Dopant Intercalation and Free Carrier Production in Sequentially Doped Conjugated Polymer Films. Advanced Functional Materials, 2020, 30, 2001800.	14.9	53
63	Dynamic Elements of Transient Spectral Hole Burning of the Hydrated Electron. The Journal of Physical Chemistry, 1994, 98, 4489-4492.	2.9	51
64	Direct observation of charge-transfer-to-solvent (CTTS) reactions: Ultrafast dynamics of the photoexcited alkali metal anion sodide (Naâ¯). Journal of Chemical Physics, 2000, 112, 9433-9444.	3.0	51
65	The Structure of the Hydrated Electron. Part 2. A Mixed Quantum/Classical Molecular Dynamics Embedded Cluster Density Functional Theory:â€‰ Singleâ¯Excitation Configuration Interaction Study. Journal of Physical Chemistry A, 2007, 111, 5232-5243.	2.5	51
66	Role of Nonpolar Forces in Aqueous Solvation:â€‰ Computer Simulation Study of Solvation Dynamics in Water Following Changes in Solute Size, Shape, and Charge. Journal of Physical Chemistry B, 1999, 103, 5570-5580.	2.6	50
67	Comparing Matched Polymer:Fullerene Solar Cells Made by Solution-Sequential Processing and Traditional Blend Casting: Nanoscale Structure and Device Performance. Journal of Physical Chemistry C, 2014, 118, 17413-17425.	3.1	50
68	Crystal Structure at 2.5 Ã... Resolution of Zinc-Substituted Copper Amine Oxidase of Hansenula polymorpha Expressed in Escherichia coli,. Biochemistry, 2000, 39, 9709-9717.	2.5	49
69	Ultrafast Studies of Exciton Migration and Polaron Formation in Sequentially Solution-Processed Conjugated Polymer/Fullerene Quasi-Bilayer Photovoltaics. Journal of Physical Chemistry Letters, 2012, 3, 2281-2287.	4.6	49
70	Electronic Structure and Transition Energies in Polymerâ€“Fullerene Bulk Heterojunctions. Journal of Physical Chemistry C, 2014, 118, 21873-21883.	3.1	48
71	Crystallinity Effects in Sequentially Processed and Blend-Cast Bulk-Heterojunction Polymer/Fullerene Photovoltaics. Journal of Physical Chemistry C, 2014, 118, 18424-18435.	3.1	46
72	Nanoscopic interchain aggregate domain formation in conjugated polymer films studied by third harmonic generation near-field scanning optical microscopy. Journal of Chemical Physics, 2002, 117, 6688-6698.	3.0	43

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73	Photo-redox activated drug delivery systems operating under two photon excitation in the near-IR. Nanoscale, 2014, 6, 4652-4658.	5.6	43
74	What makes a chromophore?. Nature Materials, 2008, 7, 427-428.	27.5	42
75	Photoinduced Charge Carrier Generation and Decay in Sequentially Deposited Polymer/Fullerene Layers: Bulk Heterojunction vs Planar Interface. Journal of Physical Chemistry C, 2012, 116, 7293-7305.	3.1	42
76	Resonance Raman and temperature-dependent electronic absorption spectra of cavity and noncavity models of the hydrated electron. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 2712-2717.	7.1	42
77	Relationship between Conserved Consensus Site Residues and the Productive Conformation for the TPQ Cofactor in a Copper-Containing Amine Oxidase from Yeast. Biochemistry, 1998, 37, 16591-16600.	2.5	41
78	Controlling the Spontaneous Precipitation of Silver Nanoparticles in Sol-Gel Materials. Journal of Sol-Gel Science and Technology, 2000, 19, 249-252.	2.4	41
79	A computationally efficient exact pseudopotential method. I. Analytic reformulation of the Phillips-Kleinman theory. Journal of Chemical Physics, 2006, 125, 074102.	3.0	41
80	Extensive Penetration of Evaporated Electrode Metals into Fullerene Films: Intercalated Metal Nanostructures and Influence on Device Architecture. ACS Applied Materials & Interfaces, 2015, 7, 25247-25258.	8.0	40
81	Controlling the Formation of Charge Transfer Complexes in Chemically Doped Semiconducting Polymers. Chemistry of Materials, 2021, 33, 2343-2356.	6.7	40
82	Solvent effects on the ultrafast dynamics and spectroscopy of the charge-transfer-to-solvent reaction of sodide. Journal of Chemical Physics, 2003, 118, 5916-5931.	3.0	38
83	An Exploration of the Relationship between Solvation Dynamics and Spectrally Determined Solvent Response Functions by Computer Simulation. The Journal of Physical Chemistry, 1995, 99, 2953-2958.	2.9	37
84	Hidden Breakdown of Linear Response:Â Projections of Molecular Motions in Nonequilibrium Simulations of Solvation Dynamics. Journal of Physical Chemistry A, 2003, 107, 4773-4777.	2.5	36
85	The role of solvent structure in the absorption spectrum of solvated electrons: Mixed quantum/classical simulations in tetrahydrofuran. Journal of Chemical Physics, 2005, 122, 134506.	3.0	36
86	Short-Range Electron Correlation Stabilizes Noncavity Solvation of the Hydrated Electron. Journal of Chemical Theory and Computation, 2016, 12, 5117-5131.	5.3	35
87	Free Energies of Cavity and Noncavity Hydrated Electrons Near the Instantaneous Air/Water Interface. Journal of Physical Chemistry Letters, 2016, 7, 3192-3198.	4.6	35
88	Ultrafast intensity-dependent stimulated emission in conjugated polymers: The mechanism for line-narrowing. Chemical Physics Letters, 1998, 288, 576-584.	2.6	34
89	Beyond PCBM: methoxylated 1,4-bisbenzyl[60]fullerene adducts for efficient organic solar cells. Journal of Materials Chemistry A, 2016, 4, 416-424.	10.3	34
90	Revisiting the pumpâ€“probe polarized transient hole-burning of the hydrated electron: Is its absorption spectrum inhomogeneously broadened?. Chemical Physics Letters, 2004, 396, 359-366.	2.6	33

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91	Understanding Nonequilibrium Solute and Solvent Motions through Molecular Projections:Â Computer Simulations of Solvation Dynamics in Liquid Tetrahydrofuran (THF). Journal of Physical Chemistry B, 2003, 107, 14464-14475.	2.6	32
92	Ultrafast Charge-Transfer-to-Solvent Dynamics of Iodide in Tetrahydrofuran. 2. Photoinduced Electron Transfer to Counterions in Solution. Journal of Physical Chemistry A, 2008, 112, 3530-3543.	2.5	32
93	Manipulating the Production and Recombination of Electrons during Electron Transfer:â€‰ Femtosecond Control of the Charge-Transfer-to-Solvent (CTTS) Dynamics of the Sodium Anion. Journal of the American Chemical Society, 2002, 124, 7622-7634.	13.7	31
94	The Ultrafast Charge-Transfer-to-Solvent Dynamics of Iodide in Tetrahydrofuran. 1. Exploring the Roles of Solvent and Solute Electronic Structure in Condensed-Phase Charge-Transfer Reactions. Journal of Physical Chemistry B, 2008, 112, 483-494.	2.6	31
95	Understanding Local and Macroscopic Electron Mobilities in the Fullerene Network of Conjugated Polymerâ€based Solar Cells: Timeâ€Resolved Microwave Conductivity and Theory. Advanced Functional Materials, 2014, 24, 784-792.	14.9	31
96	The role of electronic symmetry in charge-transfer-to-solvent reactions: Quantum nonadiabatic computer simulation of photoexcited sodium anions. Journal of Chemical Physics, 2003, 119, 11263-11277.	3.0	29
97	Watching Na Atoms Solvate into (Na+,e-) Contact Pairs:â€‰ Untangling the Ultrafast Charge-Transfer-to-Solvent Dynamics of Na- in Tetrahydrofuran (THF). Journal of Physical Chemistry A, 2007, 111, 5144-5157.	2.5	29
98	Solvents can control solute molecular identity. Nature Chemistry, 2018, 10, 910-916.	13.6	29
99	Ultrafast transient absorption spectroscopy of doped P3HT films: distinguishing free and trapped polarons. Faraday Discussions, 2019, 216, 339-362.	3.2	28
100	Calculated photon echo signals for the aqueous solvated electron. Chemical Physics Letters, 1994, 229, 443-448.	2.6	27
101	The roles of electronic exchange and correlation in charge-transfer-to-solvent dynamics: Many-electron nonadiabatic mixed quantum/classical simulations of photoexcited sodium anions in the condensed phase. Journal of Chemical Physics, 2008, 129, 164505.	3.0	27
102	Nanometer-Scale Phase Separation and Preferential Solvation in THFâ€“Water Mixtures: Ultrafast Electron Hydration and Recombination Dynamics Following CTTS Excitation of I^{â€“}. Journal of Physical Chemistry Letters, 2011, 2, 2797-2804.	4.6	26
103	Ultrafast Studies of Excess Electrons in Liquid Acetonitrile: Revisiting the Solvated Electron/Solvent Dimer Anion Equilibrium. Journal of Physical Chemistry B, 2013, 117, 4216-4221.	2.6	26
104	Self-Assembling Semiconducting Polymersâ€”Rods and Gels from Electronic Materials. ACS Nano, 2013, 7, 962-977.	14.6	25
105	Quantum decoherence: a consistent histories treatment of condensed-phase non-adiabatic quantum molecular dynamics. Computational and Theoretical Chemistry, 1997, 389, 203-216.	1.5	24
106	Time-Resolved Photoelectron Spectroscopy of the Hydrated Electron: Comparing Cavity and Noncavity Models to Experiment. Journal of Physical Chemistry B, 2016, 120, 12604-12614.	2.6	24
107	Excited state spectra and dynamics of phenyl-substituted butadienes. The Journal of Physical Chemistry, 1994, 98, 60-67.	2.9	23
108	Mapping out the conduction band under CTTS transitions: the photodetachment quantum yield of sodide (Naâ^) in tetrahydrofuran. Chemical Physics Letters, 2003, 375, 435-443.	2.6	23

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109	Using Pentaarylfullerenes to Understand Network Formation in Conjugated Polymer-Based Bulk-Heterojunction Solar Cells. Journal of Physical Chemistry C, 2011, 115, 22563-22571.	3.1	22
110	Temperature dependence of the hydrated electronâ€™s excited-state relaxation. I. Simulation predictions of resonance Raman and pump-probe transient absorption spectra of cavity and non-cavity models. Journal of Chemical Physics, 2017, 147, 074503.	3.0	22
111	A new route to dual fluorescence: Spectroscopic properties of the valence tautomers of a 3-(2H)-isoquinolinone derivative. Chemical Physics Letters, 2009, 477, 319-324.	2.6	21
112	How Does a Solvent Affect Chemical Bonds? Mixed Quantum/Classical Simulations with a Full CI Treatment of the Bonding Electrons. Journal of Physical Chemistry Letters, 2010, 1, 165-169.	4.6	21
113	Driving Force and Optical Signatures of Bipolaron Formation in Chemically Doped Conjugated Polymers. Advanced Materials, 2021, 33, e2000228.	21.0	21
114	The Molecular Basis of Solvent Caging. , 1994, , 235-248.		21
115	Nature of Sodium Atoms/(Na⁺, e^{â^'}) Contact Pairs in Liquid Tetrahydrofuran. Journal of Physical Chemistry B, 2010, 114, 11535-11543.	2.6	20
116	Nature of Excess Electrons in Polar Fluids: Anion-Solvated Electron Equilibrium and Polarized Hole-Burning in Liquid Acetonitrile. Journal of Physical Chemistry Letters, 2013, 4, 1471-1476.	4.6	20
117	Theory of Current Transients in Planar Semiconductor Devices: Insights and Applications to Organic Solar Cells. Physical Review Applied, 2015, 3, .	3.8	20
118	The interplay of dielectric and mechanical relaxation in solvation dynamics. Journal of Molecular Liquids, 1995, 65-66, 23-30.	4.9	19
119	First principles multielectron mixed quantum/classical simulations in the condensed phase. I. An efficient Fourier-grid method for solving the many-electron problem. Journal of Chemical Physics, 2010, 132, 144101.	3.0	19
120	Crystal-Packing Trends for a Series of 6,9,12,15,18-Pentaaryl-1-hydro[60]fullerenes. Chemistry - A European Journal, 2012, 18, 7418-7433.	3.3	19
121	Panoramic View of Electrochemical Pseudocapacitor and Organic Solar Cell Research in Molecularly Engineered Energy Materials (MEEM). Journal of Physical Chemistry C, 2014, 118, 19505-19523.	3.1	19
122	Moving solvated electrons with light: Nonadiabatic mixed quantum/classical molecular dynamics simulations of the relocalization of photoexcited solvated electrons in tetrahydrofuran (THF). Journal of Chemical Physics, 2006, 125, 194509.	3.0	18
123	Synthesis and Color Tuning Properties of Blue Highly Fluorescent Vinyl Polymers Containing a Pendant Pyrrolopyridazine. Macromolecules, 2005, 38, 4698-4704.	4.8	17
124	Full Configuration Interaction Computer Simulation Study of the Thermodynamic and Kinetic Stability of Hydrated Dielectrons. Journal of Physical Chemistry B, 2006, 110, 1006-1014.	2.6	17
125	Ionic strength and solvent control over the physical structure, electronic properties and superquenching of conjugated polyelectrolytes. Research on Chemical Intermediates, 2007, 33, 125-142.	2.7	17
126	Second-harmonic generation in conjugated polymer films: A sensitive probe of how bulk polymer crystallinity changes with spin speed. Journal of Chemical Physics, 2010, 133, 044901.	3.0	17

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127	Low-Vapor-Pressure Solvent Additives Function as Polymer Swelling Agents in Bulk Heterojunction Organic Photovoltaics. Journal of Physical Chemistry C, 2018, 122, 16574-16588.	3.1	17
128	Mixed Quantum/Classical Molecular Dynamics Simulations of the Hydrated Dielectron:â€‰ The Role of Exchange in Condensed-Phase Structure, Dynamics, and Spectroscopy. Journal of Physical Chemistry B, 2004, 108, 11760-11773.	2.6	16
129	Temperature dependence of the hydrated electronâ€™s excited-state relaxation. II. Elucidating the relaxation mechanism through ultrafast transient absorption and stimulated emission spectroscopy. Journal of Chemical Physics, 2017, 147, 074504.	3.0	16
130	Efficient real-space configuration-interaction method for the simulation of multielectron mixed quantum and classical nonadiabatic molecular dynamics in the condensed phase. Journal of Chemical Physics, 2003, 119, 7672-7684.	3.0	15
131	Watching the Solvation of Atoms in Liquids One Solvent Molecule at a Time. Physical Review Letters, 2010, 104, 233005.	7.8	15
132	Free Energies of Quantum Particles: The Coupled-Perturbed Quantum Umbrella Sampling Method. Journal of Chemical Theory and Computation, 2014, 10, 4661-4671.	5.3	15
133	On the insensitivity of the non-adiabatic relaxation of solvated electrons to the details of their local solvent environment. Chemical Physics Letters, 2002, 360, 22-30.	2.6	14
134	Destruction of amplified spontaneous emission via chemical doping at low-work-function metal/conjugated polymer interfaces. Applied Physics Letters, 2007, 90, 091106.	3.3	14
135	Comment on â€œAn electron-water pseudopotential for condensed phase simulationâ€•[J. Chem. Phys. 86, 3462 (1987)]. Journal of Chemical Physics, 2009, 131, 037101; author reply 037102.	3.0	14
136	Structure and Conductivity of Semiconducting Polymer Hydrogels. Journal of Physical Chemistry B, 2016, 120, 6215-6224.	2.6	14
137	Understanding How Polymer Properties Control OPV Device Performance: Regioregularity, Swelling, and Morphology Optimization Using Random Poly(3-butylthiophene-co-3-octylthiophene) Polymers. Journal of Physical Chemistry C, 2016, 120, 22115-22125.	3.1	14
138	Processing Methods for Obtaining a Face-On Crystalline Domain Orientation in Conjugated Polymer-Based Photovoltaics. Journal of Physical Chemistry C, 2018, 122, 15078-15089.	3.1	14
139	The Fluxional Nature of the Hydrated Electron: Energy and Entropy Contributions to Aqueous Electron Free Energies. Journal of Chemical Theory and Computation, 2020, 16, 1263-1270.	5.3	14
140	Evaluating Simple Ab Initio Models of the Hydrated Electron: The Role of Dynamical Fluctuations. Journal of Physical Chemistry B, 2020, 124, 9592-9603.	2.6	14
141	Stygobiont Diversity in the San Marcos Artesian Well and Edwards Aquifer Groundwater Ecosystem, Texas, USA. Diversity, 2021, 13, 234.	1.7	14
142	Directional energy migration in an oriented nanometer-scale host/guest composite: semiconducting polymers threaded into mesoporous silica. Microporous and Mesoporous Materials, 2001, 44-45, 445-451.	4.4	13
143	A computationally efficient exact pseudopotential method. II. Application to the molecular pseudopotential of an excess electron interacting with tetrahydrofuran (THF). Journal of Chemical Physics, 2006, 125, 074103.	3.0	13
144	Ultrafast dynamics of sterically hindered tetraphenylmethylbutadiene in liquids. Chemical Physics Letters, 1995, 235, 471-478.	2.6	12

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145	Higher efficiency conjugated polymer-based LEDs by control of polymer film morphology and interchain interactions. Synthetic Metals, 2001, 119, 523-524.	3.9	12
146	Nonadiabatic Molecular Dynamics Simulations of Correlated Electrons in Solution. 1. Full Configuration Interaction (CI) Excited-State Relaxation Dynamics of Hydrated Dielectrons. Journal of Physical Chemistry B, 2006, 110, 9681-9691.	2.6	12
147	Projections of Quantum Observables onto Classical Degrees of Freedom in Mixed Quantum-Classical Simulations: Understanding Linear Response Failure for the Photoexcited Hydrated Electron. Physical Review Letters, 2006, 97, 130403.	7.8	12
148	Searching for solvent cavities via electron photodetachment: The ultrafast charge-transfer-to-solvent dynamics of sodide in a series of ether solvents. Journal of Chemical Physics, 2009, 131, 154506.	3.0	12
149	Quantifying Potential Recharge in Mantled Sinkholes Using ERT. Ground Water, 2009, 47, 370-381.	1.3	12
150	First principles multielectron mixed quantum/classical simulations in the condensed phase. II. The charge-transfer-to-solvent states of sodium anions in liquid tetrahydrofuran. Journal of Chemical Physics, 2010, 132, 144102.	3.0	12
151	Elucidating the initial dynamics of electron photodetachment from atoms in liquids using variably-time-delayed resonant multiphoton ionization. Journal of Chemical Physics, 2004, 121, 374.	3.0	11
152	Nonadiabatic Molecular Dynamics Simulations of Correlated Electrons in Solution. 2. A Prediction for the Observation of Hydrated Dielectrons with Pumpâ^'Probe Spectroscopy. Journal of Physical Chemistry B, 2006, 110, 9692-9697.	2.6	11
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