

# Benjamin F Schwartz

## List of Publications by Year in descending order

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189  
papers

12,516  
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26630

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192  
docs citations

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times ranked

10132  
citing authors

#	ARTICLE	IF	CITATIONS
1	Hydrated Electrons in High-Concentration Electrolytes Interact with Multiple Cations: A Simulation Study. <i>Journal of Physical Chemistry B</i> , 2022, 126, 3748-3757.	2.6	9
2	Molecular Dynamics Study of the Thermodynamics of Integer Charge Transfer vs Charge-Transfer Complex Formation in Doped Conjugated Polymers. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 26988-27001.	8.0	11
3	Understanding the Temperature Dependence and Finite Size Effects in Ab Initio MD Simulations of the Hydrated Electron. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4973-4982.	5.3	10
4	Driving Force and Optical Signatures of Bipolaron Formation in Chemically Doped Conjugated Polymers. <i>Advanced Materials</i> , 2021, 33, e2000228.	21.0	21
5	Controlling the Formation of Charge Transfer Complexes in Chemically Doped Semiconducting Polymers. <i>Chemistry of Materials</i> , 2021, 33, 2343-2356.	6.7	40
6	New stygofauna from Texas, USA: three new species of Parabathynellidae (Crustacea: Bathynellacea). <i>Journal of Natural History</i> , 2021, 55, 979-1007.	0.5	3
7	Stygobiont Diversity in the San Marcos Artesian Well and Edwards Aquifer Groundwater Ecosystem, Texas, USA. <i>Diversity</i> , 2021, 13, 234.	1.7	14
8	Ab Initio Simulations of Poorly and Well Equilibrated (CH <sub>3</sub> CN) <sup>-</sup> Cluster Anions: Assigning Experimental Photoelectron Peaks to Surface-Bound Electrons and Solvated Monomer and Dimer Anions. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7685-7693.	2.5	1
9	Understanding the Effects of Confinement and Crystallinity on HJ-Coupling in Conjugated Polymers via Alignment and Isolation in an Oriented Mesoporous Silica Host. <i>Journal of Physical Chemistry C</i> , 2021, 125, 23240-23249.	3.1	4
10	Vibrational Stark Effect Mapping of Polaron Delocalization in Chemically Doped Conjugated Polymers. <i>Chemistry of Materials</i> , 2021, 33, 8489-8500.	6.7	10
11	How Water <sup>-</sup> Ion Interactions Control the Formation of Hydrated Electron:Sodium Cation Contact Pairs. <i>Journal of Physical Chemistry B</i> , 2021, 125, 13027-13040.	2.6	10
12	Three new microcerberids (Isopoda: Microcerberidae) from subterranean freshwater habitats in Texas, USA. <i>Journal of Natural History</i> , 2021, 55, 2261-2278.	0.5	0
13	The Fluxional Nature of the Hydrated Electron: Energy and Entropy Contributions to Aqueous Electron Free Energies. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1263-1270.	5.3	14
14	Evaluating Simple <i>Ab Initio</i> Models of the Hydrated Electron: The Role of Dynamical Fluctuations. <i>Journal of Physical Chemistry B</i> , 2020, 124, 9592-9603.	2.6	14
15	Environmental influences on invertebrate diversity and community composition in the hyporheic zone ecotone in Texas, USA: contrasts between co-occurring epigeic taxa and stygobionts. <i>Hydrobiologia</i> , 2020, 847, 3967-3982.	2.0	8
16	The Role of the Solvent in the Condensed-Phase Dynamics and Identity of Chemical Bonds: The Case of the Sodium Dimer Cation in THF. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6603-6616.	2.6	9
17	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. <i>Advanced Functional Materials</i> , 2020, 30, 2001800.	14.9	53
18	Nonequilibrium Solvent Effects during Photodissociation in Liquids: Dynamical Energy Surfaces, Caging, and Chemical Identity. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 9230-9238.	4.6	7

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19	Dopant-Induced Ordering of Amorphous Regions in Regiorandom P3HT. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4929-4934.	4.6	63
20	The <i>JPC</i> Periodic Table. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5837-5848.	2.5	2
21	The <i>JPC</i> Periodic Table. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5973-5984.	2.6	1
22	The <i>JPC</i> Periodic Table. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4051-4062.	4.6	2
23	Evaporation vs Solution Sequential Doping of Conjugated Polymers: F <sub>4</sub> TCNQ Doping of Micrometer-Thick P3HT Films for Thermoelectrics. <i>Journal of Physical Chemistry C</i> , 2019, 123, 22711-22724.	3.1	55
24	Ultrafast transient absorption spectroscopy of doped P3HT films: distinguishing free and trapped polarons. <i>Faraday Discussions</i> , 2019, 216, 339-362.	3.2	28
25	Dodecaborane-Based Dopants Designed to Shield Anion Electrostatics Lead to Increased Carrier Mobility in a Doped Conjugated Polymer. <i>Advanced Materials</i> , 2019, 31, e1805647.	21.0	90
26	<i>Cirolanides wassenichae</i> sp. nov., a freshwater, subterranean Cirolanidae (Isopoda, Cymothoidea) with additional records of other species from Texas, United States. <i>Zootaxa</i> , 2019, 4543, 498.	0.5	3
27	Bay-Linked Perylenediimides are Two Molecules in One: Insights from Ultrafast Spectroscopy, Temperature Dependence, and Time-Dependent Density Functional Theory Calculations. <i>Journal of Physical Chemistry C</i> , 2019, 123, 2127-2138.	3.1	8
28	Designing Conjugated Polymers for Molecular Doping: The Roles of Crystallinity, Swelling, and Conductivity in Sequentially-Doped Selenophene-Based Copolymers. <i>Chemistry of Materials</i> , 2019, 31, 73-82.	6.7	56
29	Description of a new genus and species of Bathynellidae (Crustacea: Bathynellacea) from Texas based on morphological and molecular characters. <i>Journal of Natural History</i> , 2018, 52, 29-51.	0.5	5
30	Thermal Equilibration Controls H-Bonding and the Vertical Detachment Energy of Water Cluster Anions. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5173-5178.	4.6	11
31	Solvents can control solute molecular identity. <i>Nature Chemistry</i> , 2018, 10, 910-916.	13.6	29
32	Low-Vapor-Pressure Solvent Additives Function as Polymer Swelling Agents in Bulk Heterojunction Organic Photovoltaics. <i>Journal of Physical Chemistry C</i> , 2018, 122, 16574-16588.	3.1	17
33	Processing Methods for Obtaining a Face-On Crystalline Domain Orientation in Conjugated Polymer-Based Photovoltaics. <i>Journal of Physical Chemistry C</i> , 2018, 122, 15078-15089.	3.1	14
34	Sequential Processing: A Rational Route for Bulk Heterojunction Formation via Polymer Swelling. <i>Materials and Energy</i> , 2018, , 309-348.	0.1	1
35	<i>Lacrimacandona</i> n. gen. (Crustacea: Ostracoda: Candonidae) from the Edwards Aquifer, Texas (USA). <i>Zootaxa</i> , 2017, 4277, 261.	0.5	6
36	The Effects of Crystallinity on Charge Transport and the Structure of Sequentially Processed F <sub>4</sub> TCNQ-Doped Conjugated Polymer Films. <i>Advanced Functional Materials</i> , 2017, 27, 1702654.	14.9	190

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37	New Physical Insights for Manuscripts on Organic and Perovskite-based Photovoltaics (and Other) Tj ETQq1 1 0.784314 rgBT <sub>0</sub> /Overlo	3.1	14
38	Temperature dependence of the hydrated electron's excited-state relaxation. II. Elucidating the relaxation mechanism through ultrafast transient absorption and stimulated emission spectroscopy. <i>Journal of Chemical Physics</i> , 2017, 147, 074504.	3.0	16
39	Temperature dependence of the hydrated electron's excited-state relaxation. I. Simulation predictions of resonance Raman and pump-probe transient absorption spectra of cavity and non-cavity models. <i>Journal of Chemical Physics</i> , 2017, 147, 074503.	3.0	22
40	Short-Range Electron Correlation Stabilizes Noncavity Solvation of the Hydrated Electron. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5117-5131.	5.3	35
41	Time-Resolved Photoelectron Spectroscopy of the Hydrated Electron: Comparing Cavity and Noncavity Models to Experiment. <i>Journal of Physical Chemistry B</i> , 2016, 120, 12604-12614.	2.6	24
42	Structure and Conductivity of Semiconducting Polymer Hydrogels. <i>Journal of Physical Chemistry B</i> , 2016, 120, 6215-6224.	2.6	14
43	Free Energies of Cavity and Noncavity Hydrated Electrons Near the Instantaneous Air/Water Interface. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3192-3198.	4.6	35
44	Understanding How Polymer Properties Control OPV Device Performance: Regioregularity, Swelling, and Morphology Optimization Using Random Poly(3-butylthiophene- <i>co</i> -3-octylthiophene) Polymers. <i>Journal of Physical Chemistry C</i> , 2016, 120, 22115-22125.	3.1	14
45	Drift-Diffusion Studies of Compositional Morphology in Bulk Heterojunctions: The Role of the Mixed Phase in Photovoltaic Performance. <i>Physical Review Applied</i> , 2016, 6, .	3.8	11
46	Discovery of a Novel 2,6-Disubstituted Glucosamine Series of Potent and Selective Hexokinase 2 Inhibitors. <i>ACS Medicinal Chemistry Letters</i> , 2016, 7, 217-222.	2.8	64
47	Beyond PCBM: methoxylated 1,4-bisbenzyl[60]fullerene adducts for efficient organic solar cells. <i>Journal of Materials Chemistry A</i> , 2016, 4, 416-424.	10.3	34
48	Drift-Diffusion Modeling of the Effects of Structural Disorder and Carrier Mobility on the Performance of Organic Photovoltaic Devices. <i>Physical Review Applied</i> , 2015, 4, .	3.8	7
49	Sequential Processing for Organic Photovoltaics: Design Rules for Morphology Control by Tailored Semi-Orthogonal Solvent Blends. <i>Advanced Energy Materials</i> , 2015, 5, 1402020.	19.5	82
50	Long-lived photoinduced polaron formation in conjugated polyelectrolyte-fullerene assemblies. <i>Science</i> , 2015, 348, 1340-1343.	12.6	53
51	Theory of Current Transients in Planar Semiconductor Devices: Insights and Applications to Organic Solar Cells. <i>Physical Review Applied</i> , 2015, 3, .	3.8	20
52	Extensive Penetration of Evaporated Electrode Metals into Fullerene Films: Intercalated Metal Nanostructures and Influence on Device Architecture. <i>ACS Applied Materials &amp; Interfaces</i> , 2015, 7, 25247-25258.	8.0	40
53	Overcoming Film Quality Issues for Conjugated Polymers Doped with F <sub>4</sub> TCNQ by Solution Sequential Processing: Hall Effect, Structural, and Optical Measurements. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4786-4793.	4.6	175
54	Understanding Local and Macroscopic Electron Mobilities in the Fullerene Network of Conjugated Polymer-based Solar Cells: Time-Resolved Microwave Conductivity and Theory. <i>Advanced Functional Materials</i> , 2014, 24, 784-792.	14.9	31

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55	Photo-redox activated drug delivery systems operating under two photon excitation in the near-IR. <i>Nanoscale</i> , 2014, 6, 4652-4658.	5.6	43
56	Panoramic View of Electrochemical Pseudocapacitor and Organic Solar Cell Research in Molecularly Engineered Energy Materials (MEEM). <i>Journal of Physical Chemistry C</i> , 2014, 118, 19505-19523.	3.1	19
57	Crystallinity Effects in Sequentially Processed and Blend-Cast Bulk-Heterojunction Polymer/Fullerene Photovoltaics. <i>Journal of Physical Chemistry C</i> , 2014, 118, 18424-18435.	3.1	46
58	Free Energies of Quantum Particles: The Coupled-Perturbed Quantum Umbrella Sampling Method. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4661-4671.	5.3	15
59	Comparing Matched Polymer:Fullerene Solar Cells Made by Solution-Sequential Processing and Traditional Blend Casting: Nanoscale Structure and Device Performance. <i>Journal of Physical Chemistry C</i> , 2014, 118, 17413-17425.	3.1	50
60	Electronic Structure and Transition Energies in Polymer-Fullerene Bulk Heterojunctions. <i>Journal of Physical Chemistry C</i> , 2014, 118, 21873-21883.	3.1	48
61	Activation of Snap-Top Capped Mesoporous Silica Nanocontainers Using Two Near-Infrared Photons. <i>Journal of the American Chemical Society</i> , 2013, 135, 14000-14003.	13.7	132
62	Resonance Raman and temperature-dependent electronic absorption spectra of cavity and noncavity models of the hydrated electron. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 2712-2717.	7.1	42
63	Ultrafast Studies of Excess Electrons in Liquid Acetonitrile: Revisiting the Solvated Electron/Solvent Dimer Anion Equilibrium. <i>Journal of Physical Chemistry B</i> , 2013, 117, 4216-4221.	2.6	26
64	Self-Assembling Semiconducting Polymers-Rods and Gels from Electronic Materials. <i>ACS Nano</i> , 2013, 7, 962-977.	14.6	25
65	Nature of Excess Electrons in Polar Fluids: Anion-Solvated Electron Equilibrium and Polarized Hole-Burning in Liquid Acetonitrile. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1471-1476.	4.6	20
66	Response to "Comment on "Going beyond the frozen core approximation: Development of coordinate-dependent pseudopotentials and application to $\text{Na}^{2+}$ ". [J. Chem. Phys. 139, 147101 (2013)]. <i>Journal of Chemical Physics</i> , 2013, 139, 147102.	3.0	0
67	To Be or Not to Be in a Cavity: The Hydrated Electron Dilemma. <i>Journal of Physical Chemistry B</i> , 2013, 117, 14173-14182.	2.6	58
68	Going beyond the frozen core approximation: Development of coordinate-dependent pseudopotentials and application to $\text{Na}^{2+}$ . <i>Journal of Chemical Physics</i> , 2013, 138, 054110.	3.0	8
69	Photoinduced Charge Carrier Generation and Decay in Sequentially Deposited Polymer/Fullerene Layers: Bulk Heterojunction vs Planar Interface. <i>Journal of Physical Chemistry C</i> , 2012, 116, 7293-7305.	3.1	42
70	Ultrafast Studies of Exciton Migration and Polaron Formation in Sequentially Solution-Processed Conjugated Polymer/Fullerene Quasi-Bilayer Photovoltaics. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2281-2287.	4.6	49
71	Crystal-Packing Trends for a Series of 6,9,12,15,18-Pentaaryl-1-hydro[60]fullerenes. <i>Chemistry - A European Journal</i> , 2012, 18, 7418-7433.	3.3	19
72	Simulating the Formation of Sodium:Electron Tight-Contact Pairs: Watching the Solvation of Atoms in Liquids One Molecule at a Time. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5887-5894.	2.5	11

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73	Nanometer-Scale Phase Separation and Preferential Solvation in THF/Water Mixtures: Ultrafast Electron Hydration and Recombination Dynamics Following CTTS Excitation of I <sup>+</sup> . Journal of Physical Chemistry Letters, 2011, 2, 2797-2804.	4.6	26
74	Charge-carrier dynamics in hybrid plasmonic organic solar cells with Ag nanoparticles. Applied Physics Letters, 2011, 98, .	3.3	138
75	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
76	Response to Comments on "Does the Hydrated Electron Occupy a Cavity?". Science, 2011, 331, 1387-1387.	12.6	58
77	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
78	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
79	Watching the Solvation of Atoms in Liquids One Solvent Molecule at a Time. Physical Review Letters, 2010, 104, 233005.	7.8	15
80	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
81	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
82	Does the Hydrated Electron Occupy a Cavity?. Science, 2010, 329, 65-69.	12.6	212
83	Hybrid conjugated polymer solar cells using patterned GaAs nanopillars. Applied Physics Letters, 2010, 97, 013107.	3.3	60
84	Nature of Sodium Atoms/(Na <sup>+</sup> , e <sup>-</sup> ) Contact Pairs in Liquid Tetrahydrofuran. Journal of Physical Chemistry B, 2010, 114, 11535-11543.	2.6	20
85	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
86	Quantifying Potential Recharge in Mantled Sinkholes Using ERT. Ground Water, 2009, 47, 370-381.	1.3	12
87	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
88	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
89	Comment on "An electron-water pseudopotential for condensed phase simulation". J. Chem. Phys. 86, 3462 (1987)]. Journal of Chemical Physics, 2009, 131, 037101; author reply 037102.	3.0	14
90	Reappraising the Need for Bulk Heterojunctions in Polymer/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

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91	What makes a chromophore?. <i>Nature Materials</i> , 2008, 7, 427-428.	27.5	42
92	Quantifying field-scale soil moisture using electrical resistivity imaging. <i>Journal of Hydrology</i> , 2008, 362, 234-246.	5.4	96
93	The roles of the solute and solvent cavities in charge-transfer-to-solvent dynamics: Ultrafast studies of potassium and sodium in diethyl ether. <i>Journal of Chemical Physics</i> , 2008, 129, 134503.	3.0	8
94	Room to Improve Conjugated Polymer-Based Solar Cells: Understanding How Thermal Annealing Affects the Fullerene Component of a Bulk Heterojunction Photovoltaic Device. <i>Journal of Physical Chemistry C</i> , 2008, 112, 18711-18716.	3.1	94
95	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. <i>Journal of Physical Chemistry B</i> , 2008, 112, 483-494.	2.6	31
96	Self-Assembling Fullerenes for Improved Bulk-Heterojunction Photovoltaic Devices. <i>Journal of the American Chemical Society</i> , 2008, 130, 17290-17292.	13.7	107
97	Ultrafast Charge-Transfer-to-Solvent Dynamics of Iodide in Tetrahydrofuran. 2. Photoinduced Electron Transfer to Counterions in Solution. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3530-3543.	2.5	32
98	Linear Response Breakdown in Solvation Dynamics Induced by Atomic Electron-Transfer Reactions. <i>Science</i> , 2008, 321, 1817-1822.	12.6	65
99	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. <i>Journal of Chemical Physics</i> , 2008, 129, 164505.	3.0	27
100	Calibrating Access to Time Domain Reflectometry Soil Water Measurements in Deep Heterogeneous Soils. <i>Soil Science Society of America Journal</i> , 2008, 72, 917-930.	2.2	8
101	Destruction of amplified spontaneous emission via chemical doping at low-work-function metal/conjugated polymer interfaces. <i>Applied Physics Letters</i> , 2007, 90, 091106.	3.3	14
102	Watching Na Atoms Solvate into (Na <sup>+</sup> ,e <sup>-</sup> ) Contact Pairs: Untangling the Ultrafast Charge-Transfer-to-Solvent Dynamics of Na <sup>-</sup> in Tetrahydrofuran (THF). <i>Journal of Physical Chemistry A</i> , 2007, 111, 5144-5157.	2.5	29
103	The Structure of the Hydrated Electron. Part 2. A Mixed Quantum/Classical Molecular Dynamics Embedded Cluster Density Functional Theory: Single Excitation Configuration Interaction Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5232-5243.	2.5	51
104	Controlling optical gain in semiconducting polymers with nanoscale chain positioning and alignment. <i>Nature Nanotechnology</i> , 2007, 2, 647-652.	31.5	102
105	Ionic strength and solvent control over the physical structure, electronic properties and superquenching of conjugated polyelectrolytes. <i>Research on Chemical Intermediates</i> , 2007, 33, 125-142.	2.7	17
106	A computationally efficient exact pseudopotential method. I. Analytic reformulation of the Phillips-Kleinman theory. <i>Journal of Chemical Physics</i> , 2006, 125, 074102.	3.0	41
107	Nonadiabatic Molecular Dynamics Simulations of Correlated Electrons in Solution. 2. A Prediction for the Observation of Hydrated Dielectrons with Pump-Probe Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2006, 110, 9692-9697.	2.6	11
108	Full Configuration Interaction Computer Simulation Study of the Thermodynamic and Kinetic Stability of Hydrated Dielectrons. <i>Journal of Physical Chemistry B</i> , 2006, 110, 1006-1014.	2.6	17

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109	Nonadiabatic Molecular Dynamics Simulations of Correlated Electrons in Solution. 1. Full Configuration Interaction (CI) Excited-State Relaxation Dynamics of Hydrated Dielectrons. <i>Journal of Physical Chemistry B</i> , 2006, 110, 9681-9691.	2.6	12
110	Exploring the Role of Decoherence in Condensed-Phase Nonadiabatic Dynamics: A Comparison of Different Mixed Quantum/Classical Simulation Algorithms for the Excited Hydrated Electron. <i>Journal of Physical Chemistry B</i> , 2006, 110, 20055-20066.	2.6	62
111	Moving solvated electrons with light: Nonadiabatic mixed quantum/classical molecular dynamics simulations of the relocalization of photoexcited solvated electrons in tetrahydrofuran (THF). <i>Journal of Chemical Physics</i> , 2006, 125, 194509.	3.0	18
112	A computationally efficient exact pseudopotential method. II. Application to the molecular pseudopotential of an excess electron interacting with tetrahydrofuran (THF). <i>Journal of Chemical Physics</i> , 2006, 125, 074103.	3.0	13
113	Projections of Quantum Observables onto Classical Degrees of Freedom in Mixed Quantum-Classical Simulations: Understanding Linear Response Failure for the Photoexcited Hydrated Electron. <i>Physical Review Letters</i> , 2006, 97, 130403.	7.8	12
114	Synthesis and Color Tuning Properties of Blue Highly Fluorescent Vinyl Polymers Containing a Pendant Pyrrolopyridazine. <i>Macromolecules</i> , 2005, 38, 4698-4704.	4.8	17
115	Mean-field dynamics with stochastic decoherence (MF-SD): A new algorithm for nonadiabatic mixed quantum/classical molecular-dynamics simulations with nuclear-induced decoherence. <i>Journal of Chemical Physics</i> , 2005, 123, 234106.	3.0	181
116	The role of solvent structure in the absorption spectrum of solvated electrons: Mixed quantum/classical simulations in tetrahydrofuran. <i>Journal of Chemical Physics</i> , 2005, 122, 134506.	3.0	36
117	Exciton-exciton annihilation and the production of interchain species in conjugated polymer films: Comparing the ultrafast stimulated emission and photoluminescence dynamics of MEH-PPV. <i>Physical Review B</i> , 2004, 69, .	3.2	120
118	Elucidating the initial dynamics of electron photodetachment from atoms in liquids using variably-time-delayed resonant multiphoton ionization. <i>Journal of Chemical Physics</i> , 2004, 121, 374.	3.0	11
119	Revisiting the pump-probe polarized transient hole-burning of the hydrated electron: Is its absorption spectrum inhomogeneously broadened?. <i>Chemical Physics Letters</i> , 2004, 396, 359-366.	2.6	33
120	Mixed Quantum/Classical Molecular Dynamics Simulations of the Hydrated Dielectron: The Role of Exchange in Condensed-Phase Structure, Dynamics, and Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2004, 108, 11760-11773.	2.6	16
121	Mapping out the conduction band under CTTS transitions: the photodetachment quantum yield of sodide (Na <sup>-</sup> ) in tetrahydrofuran. <i>Chemical Physics Letters</i> , 2003, 375, 435-443.	2.6	23
122	Understanding Nonequilibrium Solute and Solvent Motions through Molecular Projections: A Computer Simulations of Solvation Dynamics in Liquid Tetrahydrofuran (THF). <i>Journal of Physical Chemistry B</i> , 2003, 107, 14464-14475.	2.6	32
123	Hidden Breakdown of Linear Response: Projections of Molecular Motions in Nonequilibrium Simulations of Solvation Dynamics. <i>Journal of Physical Chemistry A</i> , 2003, 107, 4773-4777.	2.5	36
124	CONJUGATEDPOLYMERS ASMOLECULARMATERIALS: How Chain Conformation and Film Morphology Influence Energy Transfer and Interchain Interactions. <i>Annual Review of Physical Chemistry</i> , 2003, 54, 141-172.	10.8	901
125	The role of electronic symmetry in charge-transfer-to-solvent reactions: Quantum nonadiabatic computer simulation of photoexcited sodium anions. <i>Journal of Chemical Physics</i> , 2003, 119, 11263-11277.	3.0	29
126	Solvent effects on the ultrafast dynamics and spectroscopy of the charge-transfer-to-solvent reaction of sodide. <i>Journal of Chemical Physics</i> , 2003, 118, 5916-5931.	3.0	38



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127	Efficient real-space configuration-interaction method for the simulation of multielectron mixed quantum and classical nonadiabatic molecular dynamics in the condensed phase. <i>Journal of Chemical Physics</i> , 2003, 119, 7672-7684.	3.0	15
128	Solvent Control of Electron Transfer Dynamics. <i>Springer Series in Chemical Physics</i> , 2003, , 459-461.	0.2	5
129	Control of an electron transfer reaction using a sequence of femtosecond laser pulses. <i>Springer Series in Chemical Physics</i> , 2003, , 487-489.	0.2	3
130	Nanosopic interchain aggregate domain formation in conjugated polymer films studied by third harmonic generation near-field scanning optical microscopy. <i>Journal of Chemical Physics</i> , 2002, 117, 6688-6698.	3.0	43
131	Manipulating the Production and Recombination of Electrons during Electron Transfer: Femtosecond Control of the Charge-Transfer-to-Solvent (CTTS) Dynamics of the Sodium Anion. <i>Journal of the American Chemical Society</i> , 2002, 124, 7622-7634.	13.7	31
132	lonomeric control of interchain interactions, morphology, and the electronic properties of conjugated polymer solutions and films. <i>Journal of Chemical Physics</i> , 2002, 116, 8198-8208.	3.0	70
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134	On the insensitivity of the non-adiabatic relaxation of solvated electrons to the details of their local solvent environment. <i>Chemical Physics Letters</i> , 2002, 360, 22-30.	2.6	14
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