

# Mark A Ratner

## List of Publications by Year in descending order

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332  
papers

40,680  
citations

4120

87  
h-index

2439

197  
g-index

343  
all docs

343  
docs citations

343  
times ranked

29230  
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular rectifiers. <i>Chemical Physics Letters</i> , 1974, 29, 277-283.	1.2	3,474
2	Electron Transport in Molecular Wire Junctions. <i>Science</i> , 2003, 300, 1384-1389.	6.0	2,173
3	Design and construction of molecular assemblies with large second-order optical nonlinearities. Quantum chemical aspects. <i>Chemical Reviews</i> , 1994, 94, 195-242.	23.0	2,163
4	6-31G* basis set for third-row atoms. <i>Journal of Computational Chemistry</i> , 2001, 22, 976-984.	1.5	1,891
5	6-31G* basis set for atoms K through Zn. <i>Journal of Chemical Physics</i> , 1998, 109, 1223-1229.	1.2	1,766
6	Rylene and Related Diimides for Organic Electronics. <i>Advanced Materials</i> , 2011, 23, 268-284.	11.1	1,548
7	Contemporary Issues in Electron Transfer Research. <i>The Journal of Physical Chemistry</i> , 1996, 100, 13148-13168.	2.9	1,474
8	Design, Synthesis, and Properties of Molecule-Based Assemblies with Large Second-Order Optical Nonlinearities. <i>Angewandte Chemie International Edition in English</i> , 1995, 34, 155-173.	4.4	703
9	Covalently bonded single-molecule junctions with stable and reversible photoswitched conductivity. <i>Science</i> , 2016, 352, 1443-1445.	6.0	697
10	Hopping Transport in Conductive Heterocyclic Oligomers: Reorganization Energies and Substituent Effects. <i>Journal of the American Chemical Society</i> , 2005, 127, 2339-2350.	6.6	646
11	Molecular transport junctions: vibrational effects. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 103201.	0.7	618
12	Molecular-wire behaviour in p -phenylenevinylene oligomers. <i>Nature</i> , 1998, 396, 60-63.	13.7	614
13	Molecular Self-Assembled Monolayers and Multilayers for Organic and Unconventional Inorganic Thin-Film Transistor Applications. <i>Advanced Materials</i> , 2009, 21, 1407-1433.	11.1	556
14	Molecular electronics: Some views on transport junctions and beyond. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 8801-8808.	3.3	491
15	Using coherence to enhance function in chemical and biophysical systems. <i>Nature</i> , 2017, 543, 647-656.	13.7	477
16	From Molecules to Materials: Current Trends and Future Directions. <i>Advanced Materials</i> , 1998, 10, 1297-1336.	11.1	429
17	A brief history of molecular electronics. <i>Nature Nanotechnology</i> , 2013, 8, 378-381.	15.6	403
18	Organic solar cells: A new look at traditional models. <i>Energy and Environmental Science</i> , 2011, 4, 4410.	15.6	399

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19	Controlling Conformations of Conjugated Polymers and Small Molecules: The Role of Nonbonding Interactions. <i>Journal of the American Chemical Society</i> , 2013, 135, 10475-10483.	6.6	386
20	Exploring local currents in molecular junctions. <i>Nature Chemistry</i> , 2010, 2, 223-228.	6.6	375
21	Making a Molecular Wire: Charge and Spin Transport through para-Phenylene Oligomers. <i>Journal of the American Chemical Society</i> , 2004, 126, 5577-5584.	6.6	372
22	Time-dependent self-consistent field approximation for intramolecular energy transfer. I. Formulation and application to dissociation of van der Waals molecules. <i>Journal of Chemical Physics</i> , 1982, 77, 3022-3030.	1.2	371
23	Building Blocks for N-Type Molecular and Polymeric Electronics. Perfluoroalkyl- versus Alkyl-Functionalized Oligothiophenes ( $nT_s; n = 2\text{--}6$ ). Systematic Synthesis, Spectroscopy, Electrochemistry, and Solid-State Organization. <i>Journal of the American Chemical Society</i> , 2004, 126, 13480-13501.	6.6	362
24	Conductance of Molecular Wires: Influence of Molecule-Electrode Binding. <i>Journal of the American Chemical Society</i> , 1999, 121, 3428-3434.	6.6	349
25	Synthesis, Characterization, and Transistor Response of Semiconducting Silole Polymers with Substantial Hole Mobility and Air Stability. <i>Experiment and Theory. Journal of the American Chemical Society</i> , 2008, 130, 7670-7685.	6.6	342
26	Concepts in the design and engineering of single-molecule electronic devices. <i>Nature Reviews Physics</i> , 2019, 1, 211-230.	11.9	327
27	Building Blocks for n-Type Molecular and Polymeric Electronics. Perfluoroalkyl- versus Alkyl-Functionalized Oligothiophenes ( $nT_s; n = 2\text{--}6$ ). Systematics of Thin Film Microstructure, Semiconductor Performance, and Modeling of Majority Charge Injection in Field-Effect Transistors. <i>Journal of the American Chemical Society</i> , 2004, 126, 13859-13874.	6.6	321
28	n-Channel Polymers by Design: Optimizing the Interplay of Solubilizing Substituents, Crystal Packing, and Field-Effect Transistor Characteristics in Polymeric Bithiophene-Imide Semiconductors. <i>Journal of the American Chemical Society</i> , 2008, 130, 9679-9694.	6.6	308
29	Electron Transfer Rates in Bridged Molecular Systems 2. A Steady-State Analysis of Coherent Tunneling and Thermal Transitions. <i>Journal of Physical Chemistry B</i> , 2000, 104, 3817-3829.	1.2	298
30	Effect of Bond-Length Alternation in Molecular Wires. <i>Journal of the American Chemical Society</i> , 2002, 124, 10654-10655.	6.6	294
31	Dynamic bond percolation theory: A microscopic model for diffusion in dynamically disordered systems. I. Definition and one-dimensional case. <i>Journal of Chemical Physics</i> , 1983, 79, 3133-3142.	1.2	279
32	Nuclear Coupling and Polarization in Molecular Transport Junctions: Beyond Tunneling to Function. <i>Science</i> , 2008, 319, 1056-1060.	6.0	273
33	Efficiency Enhancement in Organic Photovoltaic Cells: Consequences of Optimizing Series Resistance. <i>Advanced Functional Materials</i> , 2010, 20, 97-104.	7.8	260
34	Bithiopheneimide-Dithienosilole/Dithienogermole Copolymers for Efficient Solar Cells: Information from Structure-Property-Device Performance Correlations and Comparison to Thieno[3,4- <i>c</i> ]pyrrole-4,6-dione Analogues. <i>Journal of the American Chemical Society</i> , 2012, 134, 18427-18439.	6.6	257
35	Conformational Gating of Long Distance Electron Transfer through Wire-like Bridges in Donor-Bridge-Acceptor Molecules. <i>Journal of the American Chemical Society</i> , 2001, 123, 7877-7886.	6.6	256
36	Metal-Free Tetrathienoacene Sensitizers for High-Performance Dye-Sensitized Solar Cells. <i>Journal of the American Chemical Society</i> , 2015, 137, 4414-4423.	6.6	243

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37	Nanoparticle, Size, Shape, and Interfacial Effects on Leakage Current Density, Permittivity, and Breakdown Strength of Metal Oxide/Polyolefin Nanocomposites: Experiment and Theory. <i>Chemistry of Materials</i> , 2010, 22, 1567-1578.	3.2	242
38	Interface Geometry and Molecular Junction Conductance: Geometric Fluctuation and Stochastic Switching. <i>Nano Letters</i> , 2005, 5, 1668-1675.	4.5	236
39	Unequal Partnership: Asymmetric Roles of Polymeric Donor and Fullerene Acceptor in Generating Free Charge. <i>Journal of the American Chemical Society</i> , 2014, 136, 2876-2884.	6.6	235
40	Molecular Rectification in a Metal/Insulator/Metal Junction Based on Self-Assembled Monolayers. <i>Journal of the American Chemical Society</i> , 2002, 124, 11730-11736.	6.6	232
41	Understanding quantum interference in coherent molecular conduction. <i>Journal of Chemical Physics</i> , 2008, 129, 054701.	1.2	232
42	Elementary steps for charge transport in DNA: thermal activation vs. tunneling. <i>Chemical Physics</i> , 2002, 275, 61-74.	0.9	221
43	Electronic motion in DNA. <i>Nature</i> , 1999, 397, 480-481.	13.7	220
44	Quantum Interference in Acyclic Systems: Conductance of Cross-Conjugated Molecules. <i>Journal of the American Chemical Society</i> , 2008, 130, 17301-17308.	6.6	219
45	Charge Hopping in Molecular Wires as a Sequence of Electron-Transfer Reactions. <i>Journal of Physical Chemistry A</i> , 2003, 107, 3970-3980.	1.1	204
46	Resonant inelastic tunneling in molecular junctions. <i>Physical Review B</i> , 2006, 73, .	1.1	204
47	Intermediate tunnelling/hopping regime in DNA charge transport. <i>Nature Chemistry</i> , 2015, 7, 221-226.	6.6	204
48	Molecular wire conductance: Electrostatic potential spatial profile. <i>Journal of Chemical Physics</i> , 2000, 112, 6834-6839.	1.2	198
49	Self-Consistent-Field Methods for Vibrational Excitations in Polyatomic Systems. <i>Advances in Chemical Physics</i> , 2007, , 97-132.	0.3	189
50	Heat conduction in molecular transport junctions. <i>Physical Review B</i> , 2007, 75, .	1.1	187
51	Intramolecular Charge Transport along Isolated Chains of Conjugated Polymers: Effect of Torsional Disorder and Polymerization Defects. <i>Journal of Physical Chemistry B</i> , 2002, 106, 7791-7795.	1.2	186
52	In Situ Catalytic Encapsulation of Core-Shell Nanoparticles Having Variable Shell Thickness: Dielectric and Energy Storage Properties of High-Permittivity Metal Oxide Nanocomposites. <i>Chemistry of Materials</i> , 2010, 22, 5154-5164.	3.2	183
53	Conformational Order in Aggregates of Conjugated Polymers. <i>Journal of the American Chemical Society</i> , 2015, 137, 6254-6262.	6.6	177
54	Conformationally Gated Switching between Superexchange and Hopping within Oligo-p-phenylene-Based Molecular Wires. <i>Journal of the American Chemical Society</i> , 2005, 127, 11842-11850.	6.6	171

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55	Ring-fusion as a perylene diimide dimer design concept for high-performance non-fullerene organic photovoltaic acceptors. <i>Chemical Science</i> , 2016, 7, 3543-3555.	3.7	168
56	High Electron Mobility in Solution-Cast and Vapor-Deposited Phenacetyl-Quaterthiophene-Based Field-Effect Transistors: A Toward N-Type Polythiophenes. <i>Journal of the American Chemical Society</i> , 2005, 127, 13476-13477.	6.6	166
57	Structural and Electrical Functionality of NiO Interfacial Films in Bulk Heterojunction Organic Solar Cells. <i>Chemistry of Materials</i> , 2011, 23, 2218-2226.	3.2	157
58	Self-assembly of ink molecules in dip-pen nanolithography: A diffusion model. <i>Journal of Chemical Physics</i> , 2001, 115, 2721-2729.	1.2	153
59	Molecule-interface coupling effects on electronic transport in molecular wires. <i>Journal of Chemical Physics</i> , 1998, 109, 5036-5043.	1.2	150
60	Controlling Electron Transfer in Donor-Bridge-Acceptor Molecules Using Cross-Conjugated Bridges. <i>Journal of the American Chemical Society</i> , 2010, 132, 15427-15434.	6.6	144
61	Correlating Electron Transport and Molecular Structure in Organic Thin Films. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 2316-2320.	7.2	141
62	Molecular Rectifiers: A New Design Based on Asymmetric Anchoring Moieties. <i>Nano Letters</i> , 2015, 15, 1577-1584.	4.5	138
63	Single Molecule Electronics: Increasing Dynamic Range and Switching Speed Using Cross-Conjugated Species. <i>Journal of the American Chemical Society</i> , 2008, 130, 17309-17319.	6.6	136
64	Ultrafast Intersystem Crossing and Spin Dynamics of Photoexcited Perylene-3,4:9,10-bis(dicarboximide) Covalently Linked to a Nitroxide Radical at Fixed Distances. <i>Journal of the American Chemical Society</i> , 2009, 131, 3700-3712.	6.6	135
65	Towards graphene molecular electronics. <i>Nature Communications</i> , 2015, 6, 6321.	5.8	135
66	A rate constant expression for charge transfer through fluctuating bridges. <i>Journal of Chemical Physics</i> , 2003, 119, 5782-5788.	1.2	133
67	Mapping the Relation between Stacking Geometries and Singlet Fission Yield in a Class of Organic Crystals. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1065-1069.	2.1	133
68	Conformational Molecular Rectifiers. <i>Nano Letters</i> , 2004, 4, 591-595.	4.5	131
69	Direct Measurement of Singlet-Triplet Splitting within Rodlike Photogenerated Radical Ion Pairs Using Magnetic Field Effects: Estimation of the Electronic Coupling for Charge Recombination. <i>Journal of Physical Chemistry A</i> , 2003, 107, 3639-3647.	1.1	127
70	Enhanced Energy Storage and Suppressed Dielectric Loss in Oxide Core-Shell Polyolefin Nanocomposites by Moderating Internal Surface Area and Increasing Shell Thickness. <i>Advanced Materials</i> , 2012, 24, 5946-5953.	11.1	127
71	The Next Breakthrough for Organic Photovoltaics?. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 77-84.	2.1	126
72	Interfering pathways in benzene: An analytical treatment. <i>Journal of Chemical Physics</i> , 2009, 131, 194704.	1.2	121

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73	The Scope and Limitations of Ternary Blend Organic Photovoltaics. <i>Advanced Energy Materials</i> , 2015, 5, 1400891.	10.2	116
74	Charge Transfer in Donor-Bridge-Acceptor Systems: Static Disorder, Dynamic Fluctuations, and Complex Kinetics. <i>Journal of Physical Chemistry C</i> , 2008, 112, 10988-11000.	1.5	114
75	On the Line Widths of Vibrational Features in Inelastic Electron Tunneling Spectroscopy. <i>Nano Letters</i> , 2004, 4, 1605-1611.	4.5	113
76	Dissociation dynamics of vibrationally excited van der Waals clusters: $I_2XY^+ \rightarrow I_2 + X + Y^+$ ( $X, Y = He, Ne$ ). <i>Journal of Chemical Physics</i> , 1983, 79, 1808-1822.	1.2	105
77	Chemical Fabrication of Heterometallic Nanogaps for Molecular Transport Junctions. <i>Nano Letters</i> , 2009, 9, 3974-3979.	4.5	105
78	Molecular Wires: Extended Coupling and Disorder Effects. <i>The Journal of Physical Chemistry</i> , 1996, 100, 8349-8355.	2.9	103
79	Algorithms for computing Franck-Condon overlap integrals. <i>International Journal of Quantum Chemistry</i> , 2000, 77, 383-392.	1.0	103
80	Gate-controlled conductance switching in DNA. <i>Nature Communications</i> , 2017, 8, 14471.	5.8	103
81	Spectroscopic Tracking of Molecular Transport Junctions Generated by Using Click Chemistry. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 5178-5181.	7.2	102
82	Exciton Migration and Cathode Quenching in Organic Light Emitting Diodes. <i>Journal of Physical Chemistry A</i> , 2000, 104, 4704-4710.	1.1	100
83	Activated Conduction in Microscopic Molecular Junctions. <i>Journal of Physical Chemistry B</i> , 2000, 104, 2790-2793.	1.2	96
84	Electron Transport through Conjugated Molecules: When the $\pi$ System Only Tells Part of the Story. <i>ChemPhysChem</i> , 2009, 10, 257-264.	1.0	96
85	Liquid meniscus condensation in dip-pen nanolithography. <i>Journal of Chemical Physics</i> , 2002, 116, 3875-3886.	1.2	94
86	Variable Temperature Mobility Analysis of n-Channel, p-Channel, and Ambipolar Organic Field-Effect Transistors. <i>Advanced Functional Materials</i> , 2010, 20, 50-58.	7.8	93
87	Inelastic tunneling effects on noise properties of molecular junctions. <i>Physical Review B</i> , 2006, 74, .	1.1	89
88	From The Cover: An agent-based approach for modeling molecular self-organization. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 255-260.	3.3	88
89	Effect of Anchoring Groups on Single Molecule Charge Transport through Porphyrins. <i>Journal of Physical Chemistry C</i> , 2013, 117, 14890-14898.	1.5	88
90	Substantial Recoverable Energy Storage in Percolative Metallic Aluminum-Polypropylene Nanocomposites. <i>Advanced Functional Materials</i> , 2013, 23, 3560-3569.	7.8	87

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91	Modeling the inelastic electron tunneling spectra of molecular wire junctions. <i>Physical Review B</i> , 2005, 72, .	1.1	86
92	Forty years of molecular electronics: Non-equilibrium heat and charge transport at the nanoscale. <i>Physica Status Solidi (B): Basic Research</i> , 2013, 250, 2249-2266.	0.7	84
93	Photodriven quantum teleportation of an electron spin state in a covalent donor-acceptor radical system. <i>Nature Chemistry</i> , 2019, 11, 981-986.	6.6	83
94	Single-Molecule Sensing of Environmental pH at an STM Break Junction and NEGF-DFT Approach. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 1098-1102.	7.2	82
95	Two-photon excited deep-red and near-infrared emissive organic co-crystals. <i>Nature Communications</i> , 2020, 11, 4633.	5.8	82
96	Entwurf, Synthese und Eigenschaften von Molekülaggregaten mit ausgeprägten nichtlinearen optischen Eigenschaften zweiter Ordnung. <i>Angewandte Chemie</i> , 1995, 107, 167-187.	1.6	81
97	Switching in Molecular Transport Junctions: Polarization Response. <i>Journal of the American Chemical Society</i> , 2007, 129, 13313-13320.	6.6	81
98	Photoinitiated multi-step charge separation and ultrafast charge transfer induced dissociation in a pyridyl-linked photosensitizer-cobaloxime assembly. <i>Energy and Environmental Science</i> , 2013, 6, 1917.	15.6	81
99	Embedding Methods for Quantum Chemistry: Applications from Materials to Life Sciences. <i>Journal of the American Chemical Society</i> , 2020, 142, 3281-3295.	6.6	81
100	Molecular Wires: Charge Transport, Mechanisms, and Control. <i>Annals of the New York Academy of Sciences</i> , 1998, 852, 22-37.	1.8	79
101	Inelastic effects in molecular junctions in the Coulomb and Kondo regimes: Nonequilibrium equation-of-motion approach. <i>Physical Review B</i> , 2007, 76, .	1.1	79
102	The Chameleonic Nature of Electron Transport through $\pi$ -Stacked Systems. <i>Journal of the American Chemical Society</i> , 2010, 132, 7887-7889.	6.6	79
103	Mesoscale molecular network formation in amorphous organic materials. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 10055-10060.	3.3	79
104	Photophysical and Morphological Implications of Single-Strand Conjugated Polymer Folding in Solution. <i>Chemistry of Materials</i> , 2016, 28, 2814-2822.	3.2	76
105	Inelastic effects in molecular junction transport: scattering and self-consistent calculations for the Seebeck coefficient. <i>Molecular Physics</i> , 2008, 106, 397-404.	0.8	74
106	Dynamics and relaxation in interacting systems: Semigroup methods. <i>Journal of Chemical Physics</i> , 1997, 106, 7036-7043.	1.2	72
107	Phase Diagram for Assembly of Biologically-Active Peptide Amphiphiles. <i>Journal of Physical Chemistry B</i> , 2008, 112, 441-447.	1.2	71
108	Conformationally Gated Rate Processes in Biological Macromolecules. <i>Journal of Physical Chemistry A</i> , 2001, 105, 5666-5678.	1.1	69



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109	Calculation of quadratic hyperpolarizabilities for organic $\pi$ electron chromophores: Molecular geometry sensitivity of second-order nonlinear optical response. <i>International Journal of Quantum Chemistry</i> , 1992, 43, 61-82.	1.0	67
110	Hydrophobically-Driven Self-Assembly: A Geometric Packing Analysis. <i>Nano Letters</i> , 2003, 3, 623-626.	4.5	65
111	Binding at molecule/gold transport interfaces. I. Geometry and bonding. <i>Journal of Chemical Physics</i> , 2003, 119, 11926-11942.	1.2	65
112	Vapor Phase Self-Assembly of Molecular Gate Dielectrics for Thin Film Transistors. <i>Journal of the American Chemical Society</i> , 2008, 130, 7528-7529.	6.6	65
113	Theoretical principles of single-molecule electronics: A chemical and mesoscopic view. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 911-924.	1.0	64
114	Quantum Interference: The Structural Dependence of Electron Transmission through Model Systems and Cross-Conjugated Molecules. <i>Journal of Physical Chemistry C</i> , 2008, 112, 16991-16998.	1.5	63
115	Vibrational states of very floppy clusters: Approximate separability and the choice of good curvilinear coordinates for XeHe <sub>2</sub> , I <sub>2</sub> He. <i>Journal of Chemical Physics</i> , 1989, 91, 1813-1823.	1.2	62
116	Dynamic Nature of the Intramolecular Electronic Coupling Mediated by a Solvent Molecule: A Computational Study. <i>Journal of the American Chemical Society</i> , 2004, 126, 2215-2224.	6.6	62
117	Pushing electrons around. <i>Nature</i> , 2000, 404, 137-138.	13.7	61
118	Charge Conduction and Breakdown Mechanisms in Self-Assembled Nanodielectrics. <i>Journal of the American Chemical Society</i> , 2009, 131, 7158-7168.	6.6	61
119	Phenacyl Thiophene and Quinone Semiconductors Designed for Solution Processability and Air Stability in High Mobility n-Channel Field Effect Transistors. <i>Chemistry - A European Journal</i> , 2010, 16, 1911-1928.	1.7	60
120	Reassessing the use of one-electron energetics in the design and characterization of organic photovoltaics. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4538.	1.3	60
121	Ultra-High-Response, Multiply Twisted Electro-optic Chromophores: Influence of $\pi$ -System Elongation and Interplanar Torsion on Hyperpolarizability. <i>Journal of the American Chemical Society</i> , 2015, 137, 12521-12538.	6.6	60
122	Spin effects on the luminescence yield of organic light emitting diodes. <i>Journal of Chemical Physics</i> , 1998, 109, 6092-6102.	1.2	59
123	Current-voltage characteristics of tunneling molecular junctions for off-resonance injection. <i>Chemical Physics</i> , 2001, 264, 365-370.	0.9	59
124	Inelastic transport in the Coulomb blockade regime within a nonequilibrium atomic limit. <i>Physical Review B</i> , 2008, 78, .	1.1	59
125	Computational Modeling of Plasmon-Enhanced Light Absorption in a Multicomponent Dye Sensitized Solar Cell. <i>Journal of Physical Chemistry C</i> , 2012, 116, 10215-10221.	1.5	59
126	Non-exponential Length Dependence of Conductance in Iodide-Terminated Oligothiophene Single-Molecule Tunneling Junctions. <i>Journal of the American Chemical Society</i> , 2016, 138, 679-687.	6.6	59



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127	A quantitative approximation for the quantum dynamics of hydrogen transfer: Transition state dynamics and decay in ClHCl <sup>+</sup> . <i>Journal of Chemical Physics</i> , 1994, 101, 1975-1987.	1.2	57
128	Molecular Dynamics Simulations of the Charge-Induced Unfolding and Refolding of Unsolvated Cytochrome c. <i>Journal of Physical Chemistry B</i> , 1999, 103, 10017-10021.	1.2	57
129	Electrostatically-Directed Self-Assembly of Cylindrical Peptide Amphiphile Nanostructures. <i>Journal of Physical Chemistry B</i> , 2004, 108, 8817-8822.	1.2	57
130	Deep-hole transfer leads to ultrafast charge migration in DNA hairpins. <i>Nature Chemistry</i> , 2016, 8, 1015-1021.	6.6	56
131	6-31G* basis set for third-row atoms. <i>Journal of Computational Chemistry</i> , 2001, 22, 976-984.	1.5	56
132	Testing the Condon Approximation for Electron Transfer via the Mulliken-Hush Model. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8566-8569.	1.1	53
133	Injection Time in the Metaloxide-Molecule Interface Calculated within the Tight-Binding Model. <i>Journal of Physical Chemistry B</i> , 2000, 104, 8498-8502.	1.2	53
134	Structure-Performance Correlations in Vapor Phase Deposited Self-Assembled Nanodielectrics for Organic Field-Effect Transistors. <i>Journal of the American Chemical Society</i> , 2009, 131, 11080-11090.	6.6	53
135	Nonequilibrium steady state transport via the reduced density matrix operator. <i>Journal of Chemical Physics</i> , 2009, 130, 144105.	1.2	52
136	Chemistry in strong laser fields: An example from methyl iodide photodissociation. <i>Journal of Chemical Physics</i> , 1992, 97, 6410-6431.	1.2	49
137	Fabrication and characterization of metal-molecule-silicon devices. <i>Applied Physics Letters</i> , 2007, 91, 033508.	1.5	48
138	Diketopyrrolopyrrole (DPP) functionalized tetrathienothiophene (TTA) small molecules for organic thin film transistors and photovoltaic cells. <i>Journal of Materials Chemistry C</i> , 2015, 3, 8932-8941.	2.7	48
139	Ï-Dimerization of viologen subunits around the core of C60 from twelve to six directions. <i>Chemical Science</i> , 2013, 4, 1462.	3.7	47
140	Quantum Chemical Analysis of Electronic Structure and n- and p-Type Charge Transport in Perfluoroarene-Modified Oligothiophene Semiconductors. <i>Journal of Physical Chemistry B</i> , 2006, 110, 24361-24370.	1.2	46
141	Modeling geminate pair dissociation in organic solar cells: high power conversion efficiencies achieved with moderate optical bandgaps. <i>Energy and Environmental Science</i> , 2012, 5, 8343.	15.6	46
142	Two-Dimensional Model for Polymer-Based Photovoltaic Cells: Numerical Simulations of Morphology Effects. <i>Journal of Physical Chemistry B</i> , 2004, 108, 4296-4307.	1.2	45
143	Semiempirical Modeling of Ag Nanoclusters: New Parameters for Optical Property Studies Enable Determination of Double Excitation Contributions to Plasmonic Excitation. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4542-4549.	1.1	45
144	Sustainable High Capacitance at High Frequencies: Metallic Aluminum-Polypropylene Nanocomposites. <i>ACS Nano</i> , 2013, 7, 396-407.	7.3	42

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145	Organic Photovoltaics: Elucidating the Ultrafast Exciton Dissociation Mechanism in Disordered Materials. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 7456-7460.	7.2	42
146	Structural and Conformational Dispersion in the Rational Design of Conjugated Polymers. <i>Macromolecules</i> , 2014, 47, 987-992.	2.2	42
147	Is Molecular Rectification Caused by Asymmetric Electrode Couplings or by a Molecular Bias Drop?. <i>Journal of Physical Chemistry C</i> , 2015, 119, 6254-6260.	1.5	41
148	A Vibrational Eigenfunction of a Protein: Anharmonic Coupled-Mode Ground and Fundamental Excited States of BPTI. <i>Journal of Physical Chemistry B</i> , 1997, 101, 1700-1706.	1.2	40
149	Scaling analysis of electron transport through metal-semiconducting carbon nanotube interfaces: Evolution from the molecular limit to the bulk limit. <i>Physical Review B</i> , 2004, 70, .	1.1	40
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