Mark A Ratner

List of Publications by Year
in descending order

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332 papers	40,680 citations	3933 88 h-index	2448 197 g-index
343 all docs	343 docs citations	343 times ranked	29230 citing authors

#	Article	IF	Citations
1	Molecular rectifiers. Chemical Physics Letters, 1974, 29, 277-283.	2.6	3,474
2	Electron Transport in Molecular Wire Junctions. Science, 2003, 300, 1384-1389.	12.6	2,173
3	Design and construction of molecular assemblies with large second-order optical nonlinearities. Quantum chemical aspects. Chemical Reviews, 1994, 94, 195-242.	47.7	2,163
4	6-31G* basis set for third-row atoms. Journal of Computational Chemistry, 2001, 22, 976-984.	3.3	1,891
5	6-31G* basis set for atoms K through Zn. Journal of Chemical Physics, 1998, 109, 1223-1229.	3.0	1,766
6	Rylene and Related Diimides for Organic Electronics. Advanced Materials, 2011, 23, 268-284.	21.0	1,548
7	Contemporary Issues in Electron Transfer Research. The Journal of Physical Chemistry, 1996, 100, 13148-13168.	2.9	1,474
8	Design, Synthesis, and Properties of Molecule-Based Assemblies with Large Second-Order Optical Nonlinearities. Angewandte Chemie International Edition in English, 1995, 34, 155-173.	4.4	703
9	Covalently bonded single-molecule junctions with stable and reversible photoswitched conductivity. Science, 2016, 352, 1443-1445.	12.6	697
10	Hopping Transport in Conductive Heterocyclic Oligomers:Â Reorganization Energies and Substituent Effects. Journal of the American Chemical Society, 2005, 127, 2339-2350.	13.7	646
11	Molecular transport junctions: vibrational effects. Journal of Physics Condensed Matter, 2007, 19, 103201.	1.8	618
12	Molecular-wire behaviour in p -phenylenevinylene oligomers. Nature, 1998, 396, 60-63.	27.8	614
13	Molecular Selfâ€Assembled Monolayers and Multilayers for Organic and Unconventional Inorganic Thinâ€Film Transistor Applications. Advanced Materials, 2009, 21, 1407-1433.	21.0	556
14	Molecular electronics: Some views on transport junctions and beyond. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 8801-8808.	7.1	491
15	Using coherence to enhance function in chemical and biophysical systems. Nature, 2017, 543, 647-656.	27.8	477
16	From Molecules to Materials: Current Trends and Future Directions. Advanced Materials, 1998, 10, 1297-1336.	21.0	429
17	A brief history of molecular electronics. Nature Nanotechnology, 2013, 8, 378-381.	31.5	403
18	Organic solar cells: A new look at traditional models. Energy and Environmental Science, 2011, 4, 4410.	30.8	399

#	Article	IF	Citations
19	Controlling Conformations of Conjugated Polymers and Small Molecules: The Role of Nonbonding Interactions. Journal of the American Chemical Society, 2013, 135, 10475-10483.	13.7	386
20	Exploring local currents in molecular junctions. Nature Chemistry, 2010, 2, 223-228.	13.6	375
21	Making a Molecular Wire:Â Charge and Spin Transport throughpara-Phenylene Oligomers. Journal of the American Chemical Society, 2004, 126, 5577-5584.	13.7	372
22	Timeâ€dependent selfâ€consistent field approximation for intramolecular energy transfer. I. Formulation and application to dissociation of van der Waals molecules. Journal of Chemical Physics, 1982, 77, 3022-3030.	3.0	371
23	Building Blocks for N-Type Molecular and Polymeric Electronics. Perfluoroalkyl- versus Alkyl-Functionalized Oligothiophenes (nTs;n= 2â^'6). Systematic Synthesis, Spectroscopy, Electrochemistry, and Solid-State Organization. Journal of the American Chemical Society, 2004, 126, 13480-13501.	13.7	362
24	Conductance of Molecular Wires:â€‰ Influence of Moleculeâ^'Electrode Binding. Journal of the American Chemical Society, 1999, 121, 3428-3434.	13.7	349
25	Synthesis, Characterization, and Transistor Response of Semiconducting Silole Polymers with Substantial Hole Mobility and Air Stability. Experiment and Theory. Journal of the American Chemical Society, 2008, 130, 7670-7685.	13.7	342
26	Concepts in the design and engineering of single-molecule electronic devices. Nature Reviews Physics, 2019, 1, 211-230.	26.6	327
27	Building Blocks for n-Type Molecular and Polymeric Electronics. Perfluoroalkyl- versus Alkyl-Functionalized Oligothiophenes (nT;n= 2â^'6). Systematics of Thin Film Microstructure, Semiconductor Performance, and Modeling of Majority Charge Injection in Field-Effect Transistors. Journal of the American Chemical Society, 2004, 126, 13859-13874.	13.7	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. Journal of the American Chemical Society, 2008, 130, 9679-9694.	13.7	308
29	Electron Transfer Rates in Bridged Molecular Systems 2. A Steady-State Analysis of Coherent Tunneling and Thermal Transitionsâ€. Journal of Physical Chemistry B, 2000, 104, 3817-3829.	2.6	298
30	Effect of Bond-Length Alternation in Molecular Wires. Journal of the American Chemical Society, 2002, 124, 10654-10655.	13.7	294
31	Dynamic bond percolation theory: A microscopic model for diffusion in dynamically disordered systems. I. Definition and oneâ€dimensional case. Journal of Chemical Physics, 1983, 79, 3133-3142.	3.0	279
32	Nuclear Coupling and Polarization in Molecular Transport Junctions: Beyond Tunneling to Function. Science, 2008, 319, 1056-1060.	12.6	273
33	Efficiency Enhancement in Organic Photovoltaic Cells: Consequences of Optimizing Series Resistance. Advanced Functional Materials, 2010, 20, 97-104.	14.9	260
34	Bithiopheneimideâ€“Dithienosilole/Dithienogermole Copolymers for Efficient Solar Cells: Information from Structureâ€“Propertyâ€“Device Performance Correlations and Comparison to Thieno[3,4-c]pyrrole-4,6-dione Analogues. Journal of the American Chemical Society, 2012, 134, 18427-18439.	13.7	257
35	Conformational Gating of Long Distance Electron Transfer through Wire-like Bridges in Donorâ^'Bridgeâ^'Acceptor Molecules. Journal of the American Chemical Society, 2001, 123, 7877-7886.	13.7	256
36	Metal-Free Tetrathienoacene Sensitizers for High-Performance Dye-Sensitized Solar Cells. Journal of the American Chemical Society, 2015, 137, 4414-4423.	13.7	243

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37	Nanoparticle, Size, Shape, and Interfacial Effects on Leakage Current Density, Permittivity, and Breakdown Strength of Metal Oxideâ^'Polyolefin Nanocomposites: Experiment and Theory. Chemistry of Materials, 2010, 22, 1567-1578.	6.7	242
38	Interface Geometry and Molecular Junction Conductance:â€‰ Geometric Fluctuation and Stochastic Switching. Nano Letters, 2005, 5, 1668-1675.	9.1	236
39	Unequal Partnership: Asymmetric Roles of Polymeric Donor and Fullerene Acceptor in Generating Free Charge. Journal of the American Chemical Society, 2014, 136, 2876-2884.	13.7	235
40	Molecular Rectification in a Metalâ^'Insulatorâ^'Metal Junction Based on Self-Assembled Monolayers. Journal of the American Chemical Society, 2002, 124, 11730-11736.	13.7	232
41	Understanding quantum interference in coherent molecular conduction. Journal of Chemical Physics, 2008, 129, 054701.	3.0	232
42	Elementary steps for charge transport in DNA: thermal activation vs. tunneling. Chemical Physics, 2002, 275, 61-74.	1.9	221
43	Electronic motion in DNA. Nature, 1999, 397, 480-481.	27.8	220
44	Quantum Interference in Acyclic Systems: Conductance of Cross-Conjugated Molecules. Journal of the American Chemical Society, 2008, 130, 17301-17308.	13.7	219
45	Charge Hopping in Molecular Wires as a Sequence of Electron-Transfer Reactions. Journal of Physical Chemistry A, 2003, 107, 3970-3980.	2.5	204
46	Resonant inelastic tunneling in molecular junctions. Physical Review B, 2006, 73, .	3.2	204
47	Intermediate tunnellingâ€“hopping regime in DNA charge transport. Nature Chemistry, 2015, 7, 221-226.	13.6	204
48	Molecular wire conductance: Electrostatic potential spatial profile. Journal of Chemical Physics, 2000, 112, 6834-6839.	3.0	198
49	Self-Consistent-Field Methods for Vibrational Excitations in Polyatomic Systems. Advances in Chemical Physics, 2007, , 97-132.	0.3	189
50	Heat conduction in molecular transport junctions. Physical Review B, 2007, 75, .	3.2	187
51	Intramolecular Charge Transport along Isolated Chains of Conjugated Polymers:â€‰ Effect of Torsional Disorder and Polymerization Defects. Journal of Physical Chemistry B, 2002, 106, 7791-7795.	2.6	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. Chemistry of Materials, 2010, 22, 5154-5164.	6.7	183
53	Conformational Order in Aggregates of Conjugated Polymers. Journal of the American Chemical Society, 2015, 137, 6254-6262.	13.7	177
54	Conformationally Gated Switching between Superexchange and Hopping within Oligo-p-phenylene-Based Molecular Wires. Journal of the American Chemical Society, 2005, 127, 11842-11850.	13.7	171

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55	Ring-fusion as a perylenediimide dimer design concept for high-performance non-fullerene organic photovoltaic acceptors. Chemical Science, 2016, 7, 3543-3555.	7.4	168
56	High Electron Mobility in Solution-Cast and Vapor-Deposited Phenacylâ^'Quaterthiophene-Based Field-Effect Transistors:Â Toward N-Type Polythiophenes. Journal of the American Chemical Society, 2005, 127, 13476-13477.	13.7	166
57	Structural and Electrical Functionality of NiO Interfacial Films in Bulk Heterojunction Organic Solar Cells. Chemistry of Materials, 2011, 23, 2218-2226.	6.7	157
58	Self-assembly of ink molecules in dip-pen nanolithography: A diffusion model. Journal of Chemical Physics, 2001, 115, 2721-2729.	3.0	153
59	Molecule-interface coupling effects on electronic transport in molecular wires. Journal of Chemical Physics, 1998, 109, 5036-5043.	3.0	150
60	Controlling Electron Transfer in Donorâ^'Bridgeâ^'Acceptor Molecules Using Cross-Conjugated Bridges. Journal of the American Chemical Society, 2010, 132, 15427-15434.	13.7	144
61	Correlating Electron Transport and Molecular Structure in Organic Thin Films. Angewandte Chemie - International Edition, 2001, 40, 2316-2320.	13.8	141
62	Molecular Rectifiers: A New Design Based on Asymmetric Anchoring Moieties. Nano Letters, 2015, 15, 1577-1584.	9.1	138
63	Single Molecule Electronics: Increasing Dynamic Range and Switching Speed Using Cross-Conjugated Species. Journal of the American Chemical Society, 2008, 130, 17309-17319.	13.7	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. Journal of the American Chemical Society, 2009, 131, 3700-3712.	13.7	135
65	Towards graphyne molecular electronics. Nature Communications, 2015, 6, 6321.	12.8	135
66	A rate constant expression for charge transfer through fluctuating bridges. Journal of Chemical Physics, 2003, 119, 5782-5788.	3.0	133
67	Mapping the Relation between Stacking Geometries and Singlet Fission Yield in a Class of Organic Crystals. Journal of Physical Chemistry Letters, 2013, 4, 1065-1069.	4.6	133
68	Conformational Molecular Rectifiers. Nano Letters, 2004, 4, 591-595.	9.1	131
69	Direct Measurement of Singletâ^'Triplet Splitting within Rodlike Photogenerated Radical Ion Pairs Using Magnetic Field Effects:â€‰ Estimation of the Electronic Coupling for Charge Recombination. Journal of Physical Chemistry A, 2003, 107, 3639-3647.	2.5	127
70	Enhanced Energy Storage and Suppressed Dielectric Loss in Oxide Coreâ€“Shellâ€“Polyolefin Nanocomposites by Moderating Internal Surface Area and Increasing Shell Thickness. Advanced Materials, 2012, 24, 5946-5953.	21.0	127
71	The Next Breakthrough for Organic Photovoltaics?. Journal of Physical Chemistry Letters, 2015, 6, 77-84.	4.6	126
72	Interfering pathways in benzene: An analytical treatment. Journal of Chemical Physics, 2009, 131, 194704.	3.0	121

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73	The Scope and Limitations of Ternary Blend Organic Photovoltaics. Advanced Energy Materials, 2015, 5, 1400891.	19.5	116
74	Charge Transfer in Donor-Bridge-Acceptor Systems: Static Disorder, Dynamic Fluctuations, and Complex Kinetics. Journal of Physical Chemistry C, 2008, 112, 10988-11000.	3.1	114
75	On the Line Widths of Vibrational Features in Inelastic Electron Tunneling Spectroscopy. Nano Letters, 2004, 4, 1605-1611.	9.1	113
76	Dissociation dynamics of vibrationally excited van der Waals clusters: I2XYâ€‰â†’â€‰I2+X+Yâ€‰(X,â€‰Y=He,â€‰Ne). Journal of Chemical Physics, 1983, 79, 1808-1822.	3.0	105
77	Chemical Fabrication of Heterometallic Nanogaps for Molecular Transport Junctions. Nano Letters, 2009, 9, 3974-3979.	9.1	105
78	Molecular Wires:Â Extended Coupling and Disorder Effects. The Journal of Physical Chemistry, 1996, 100, 8349-8355.	2.9	103
79	Algorithms for computing Franck-Condon overlap integrals. International Journal of Quantum Chemistry, 2000, 77, 383-392.	2.0	103
80	Gate-controlled conductance switching in DNA. Nature Communications, 2017, 8, 14471.	12.8	103
81	Spectroscopic Tracking of Molecular Transport Junctions Generated by Using Click Chemistry. Angewandte Chemie - International Edition, 2009, 48, 5178-5181.	13.8	102
82	Exciton Migration and Cathode Quenching in Organic Light Emitting Diodesâ€. Journal of Physical Chemistry A, 2000, 104, 4704-4710.	2.5	100
83	Activated Conduction in Microscopic Molecular Junctions. Journal of Physical Chemistry B, 2000, 104, 2790-2793.	2.6	96
84	Electron Transport through Conjugated Molecules: When the Ï€ System Only Tells Part of the Story. ChemPhysChem, 2009, 10, 257-264.	2.1	96
85	Liquid meniscus condensation in dip-pen nanolithography. Journal of Chemical Physics, 2002, 116, 3875-3886.	3.0	94
86	Variable Temperature Mobility Analysis of nâ€Channel, pâ€Channel, and Ambipolar Organic Fieldâ€Effect Transistors. Advanced Functional Materials, 2010, 20, 50-58.	14.9	93
87	Inelastic tunneling effects on noise properties of molecular junctions. Physical Review B, 2006, 74, .	3.2	89
88	From The Cover: An agent-based approach for modeling molecular self-organization. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 255-260.	7.1	88
89	Effect of Anchoring Groups on Single Molecule Charge Transport through Porphyrins. Journal of Physical Chemistry C, 2013, 117, 14890-14898.	3.1	88
90	Substantial Recoverable Energy Storage in Percolative Metallic Aluminumâ€Polypropylene Nanocomposites. Advanced Functional Materials, 2013, 23, 3560-3569.	14.9	87

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91	Modeling the inelastic electron tunneling spectra of molecular wire junctions. Physical Review B, 2005, 72, .	3.2	86
92	Forty years of molecular electronics: Nonâ€equilibrium heat and charge transport at the nanoscale. Physica Status Solidi (B): Basic Research, 2013, 250, 2249-2266.	1.5	84
93	Photodriven quantum teleportation of an electron spin state in a covalent donorâ€“acceptorâ€“radical system. Nature Chemistry, 2019, 11, 981-986.	13.6	83
94	Singleâ€Molecule Sensing of Environmental pHâ€”an STM Break Junction and NEGFâ€DFT Approach. Angewandte Chemie - International Edition, 2014, 53, 1098-1102.	13.8	82
95	Two-photon excited deep-red and near-infrared emissive organic co-crystals. Nature Communications, 2020, 11, 4633.	12.8	82
96	Entwurf, Synthese und Eigenschaften von MolekÃ¼laggregaten mit ausgeprÃgten nichtlinearen optischen Eigenschaften zweiter Ordnung. Angewandte Chemie, 1995, 107, 167-187.	2.0	81
97	Switching in Molecular Transport Junctions:â€‰ Polarization Response. Journal of the American Chemical Society, 2007, 129, 13313-13320.	13.7	81
98	Photoinitiated multi-step charge separation and ultrafast charge transfer induced dissociation in a pyridyl-linked photosensitizerâ€“cobaloxime assembly. Energy and Environmental Science, 2013, 6, 1917.	30.8	81
99	Embedding Methods for Quantum Chemistry: Applications from Materials to Life Sciences. Journal of the American Chemical Society, 2020, 142, 3281-3295.	13.7	81
100	Molecular Wires: Charge Transport, Mechanisms, and Control. Annals of the New York Academy of Sciences, 1998, 852, 22-37.	3.8	79
101	Inelastic effects in molecular junctions in the Coulomb and Kondo regimes: Nonequilibrium equation-of-motion approach. Physical Review B, 2007, 76, .	3.2	79
102	The Chameleonic Nature of Electron Transport through Ï€-Stacked Systems. Journal of the American Chemical Society, 2010, 132, 7887-7889.	13.7	79
103	Mesoscale molecular network formation in amorphous organic materials. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 10055-10060.	7.1	79
104	Photophysical and Morphological Implications of Single-Strand Conjugated Polymer Folding in Solution. Chemistry of Materials, 2016, 28, 2814-2822.	6.7	76
105	Inelastic effects in molecular junction transport: scattering and self-consistent calculations for the Seebeck coefficient. Molecular Physics, 2008, 106, 397-404.	1.7	74
106	Dynamics and relaxation in interacting systems: Semigroup methods. Journal of Chemical Physics, 1997, 106, 7036-7043.	3.0	72
107	Phase Diagram for Assembly of Biologically-Active Peptide Amphiphiles. Journal of Physical Chemistry B, 2008, 112, 441-447.	2.6	71
108	Conformationally Gated Rate Processes in Biological Macromolecules. Journal of Physical Chemistry A, 2001, 105, 5666-5678.	2.5	69

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109	Calculation of quadratic hyperpolarizabilities for organic ? electron chromophores: Molecular geometry sensitivity of second-order nonlinear optical response. International Journal of Quantum Chemistry, 1992, 43, 61-82.	2.0	67
110	Hydrophobically-Driven Self-Assembly:â€‰ A Geometric Packing Analysis. Nano Letters, 2003, 3, 623-626.	9.1	65
111	Binding at molecule/gold transport interfaces. I. Geometry and bonding. Journal of Chemical Physics, 2003, 119, 11926-11942.	3.0	65
112	Vapor Phase Self-Assembly of Molecular Gate Dielectrics for Thin Film Transistors. Journal of the American Chemical Society, 2008, 130, 7528-7529.	13.7	65
113	Theoretical principles of single-molecule electronics: A chemical and mesoscopic view. International Journal of Quantum Chemistry, 2005, 102, 911-924.	2.0	64
114	Quantum Interference: The Structural Dependence of Electron Transmission through Model Systems and Cross-Conjugated Molecules. Journal of Physical Chemistry C, 2008, 112, 16991-16998.	3.1	63
115	Vibrational states of very floppy clusters: Approximate separability and the choice of good curvilinear coordinates for XeHe2, I2He. Journal of Chemical Physics, 1989, 91, 1813-1823.	3.0	62
116	Dynamic Nature of the Intramolecular Electronic Coupling Mediated by a Solvent Molecule:â€‰ A Computational Study. Journal of the American Chemical Society, 2004, 126, 2215-2224.	13.7	62
117	Pushing electrons around. Nature, 2000, 404, 137-138.	27.8	61
118	Charge Conduction and Breakdown Mechanisms in Self-Assembled Nanodielectrics. Journal of the American Chemical Society, 2009, 131, 7158-7168.	13.7	61
119	Phenacylâ€“Thiophene and Quinone Semiconductors Designed for Solution Processability and Airâ€Stability in High Mobility nâ€Channel Fieldâ€Effect Transistors. Chemistry - A European Journal, 2010, 16, 1911-1928.	3.3	60
120	Reassessing the use of one-electron energetics in the design and characterization of organic photovoltaics. Physical Chemistry Chemical Physics, 2013, 15, 4538.	2.8	60
121	Ultra-High-Response, Multiply Twisted Electro-optic Chromophores: Influence of Ï€-System Elongation and Interplanar Torsion on Hyperpolarizability. Journal of the American Chemical Society, 2015, 137, 12521-12538.	13.7	60
122	Spin effects on the luminescence yield of organic light emitting diodes. Journal of Chemical Physics, 1998, 109, 6092-6102.	3.0	59
123	Currentâ€“voltage characteristics of tunneling molecular junctions for off-resonance injection. Chemical Physics, 2001, 264, 365-370.	1.9	59
124	Inelastic transport in the Coulomb blockade regime within a nonequilibrium atomic limit. Physical Review B, 2008, 78, .	3.2	59
125	Computational Modeling of Plasmon-Enhanced Light Absorption in a Multicomponent Dye Sensitized Solar Cell. Journal of Physical Chemistry C, 2012, 116, 10215-10221.	3.1	59
126	Non-exponential Length Dependence of Conductance in Iodide-Terminated Oligothiophene Single-Molecule Tunneling Junctions. Journal of the American Chemical Society, 2016, 138, 679-687.	13.7	59

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127	A quantitative approximation for the quantum dynamics of hydrogen transfer: Transition state dynamics and decay in ClHClâ^'. Journal of Chemical Physics, 1994, 101, 1975-1987.	3.0	57
128	Molecular Dynamics Simulations of the Charge-Induced Unfolding and Refolding of Unsolvated Cytochrome c. Journal of Physical Chemistry B, 1999, 103, 10017-10021.	2.6	57
129	Electrostatically-Directed Self-Assembly of Cylindrical Peptide Amphiphile Nanostructures. Journal of Physical Chemistry B, 2004, 108, 8817-8822.	2.6	57
130	Deep-hole transfer leads to ultrafast charge migration in DNA hairpins. Nature Chemistry, 2016, 8, 1015-1021.	13.6	56
131	6â€31G* basis set for thirdâ€row atoms. Journal of Computational Chemistry, 2001, 22, 976-984.	3.3	56
132	Testing the Condon Approximation for Electron Transfer via the Mullikenâ^'Hush Model. Journal of Physical Chemistry A, 2000, 104, 8566-8569.	2.5	53
133	Injection Time in the Metaloxideâ^'Molecule Interface Calculated within the Tight-Binding Model. Journal of Physical Chemistry B, 2000, 104, 8498-8502.	2.6	53
134	Structureâ^'Performance Correlations in Vapor Phase Deposited Self-Assembled Nanodielectrics for Organic Field-Effect Transistors. Journal of the American Chemical Society, 2009, 131, 11080-11090.	13.7	53
135	Nonequilibrium steady state transport via the reduced density matrix operator. Journal of Chemical Physics, 2009, 130, 144105.	3.0	52
136	Chemistry in strong laser fields: An example from methyl iodide photodissociation. Journal of Chemical Physics, 1992, 97, 6410-6431.	3.0	49
137	Fabrication and characterization of metal-molecule-silicon devices. Applied Physics Letters, 2007, 91, 033508.	3.3	48
138	Diketopyrrolopyrrole (DPP) functionalized tetrathienothiophene (TTA) small molecules for organic thin film transistors and photovoltaic cells. Journal of Materials Chemistry C, 2015, 3, 8932-8941.	5.5	48
139	Ï€-Dimerization of viologen subunits around the core of C60 from twelve to six directions. Chemical Science, 2013, 4, 1462.	7.4	47
140	Quantum Chemical Analysis of Electronic Structure and n- and p-Type Charge Transport in Perfluoroarene-Modified Oligothiophene Semiconductors. Journal of Physical Chemistry B, 2006, 110, 24361-24370.	2.6	46
141	Modeling geminate pair dissociation in organic solar cells: high power conversion efficiencies achieved with moderate optical bandgaps. Energy and Environmental Science, 2012, 5, 8343.	30.8	46
142	Two-Dimensional Model for Polymer-Based Photovoltaic Cells:Â Numerical Simulations of Morphology Effects. Journal of Physical Chemistry B, 2004, 108, 4296-4307.	2.6	45
143	Semiempirical Modeling of Ag Nanoclusters: New Parameters for Optical Property Studies Enable Determination of Double Excitation Contributions to Plasmonic Excitation. Journal of Physical Chemistry A, 2016, 120, 4542-4549.	2.5	45
144	Sustainable High Capacitance at High Frequencies: Metallic Aluminumâ€“Polypropylene Nanocomposites. ACS Nano, 2013, 7, 396-407.	14.6	42

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145	Organic Photovoltaics: Elucidating the Ultraâ€Fast Exciton Dissociation Mechanism in Disordered Materials. Angewandte Chemie - International Edition, 2014, 53, 7456-7460.	13.8	42
146	Structural and Conformational Dispersion in the Rational Design of Conjugated Polymers. Macromolecules, 2014, 47, 987-992.	4.8	42
147	Is Molecular Rectification Caused by Asymmetric Electrode Couplings or by a Molecular Bias Drop?. Journal of Physical Chemistry C, 2015, 119, 6254-6260.	3.1	41
148	A Vibrational Eigenfunction of a Protein:â€‰ Anharmonic Coupled-Mode Ground and Fundamental Excited States of BPTI. Journal of Physical Chemistry B, 1997, 101, 1700-1706.	2.6	40
149	Scaling analysis of electron transport through metalâ€“semiconducting carbon nanotube interfaces: Evolution from the molecular limit to the bulk limit. Physical Review B, 2004, 70, .	3.2	40
150	Interference and Molecular Transportâ€”A Dynamical View: Time-Dependent Analysis of Disubstituted Benzenes. Journal of Physical Chemistry Letters, 2014, 5, 2748-2752.	4.6	40
151	Jahn-Teller effects in metalloporphyrins and other four-fold symmetric systems. Molecular Physics, 1978, 35, 901-925.	1.7	39
152	Charge Transport across DNA-Based Three-Way Junctions. Journal of the American Chemical Society, 2015, 137, 5113-5122.	13.7	39
153	Ground state properties and optical response of LixNa4â^'x,x=0â€“4: Anabinitiostudy. Journal of Chemical Physics, 1992, 96, 4924-4933.	3.0	38
154	Weibull Analysis of Dielectric Breakdown in a Self-Assembled Nanodielectric for Organic Transistors. Journal of Physical Chemistry Letters, 2010, 1, 3292-3297.	4.6	38
155	Molecular Conduction through Adlayers: Cooperative Effects Can Help or Hamper Electron Transport. Nano Letters, 2011, 11, 4693-4696.	9.1	38
156	Chain Length Dependence of the Dielectric Constant and Polarizability in Conjugated Organic Thin Films. ACS Nano, 2017, 11, 5970-5981.	14.6	38
157	The screened INDO (INDO/S) model: Application to photoelectron spectrum of benzonitrile. Journal of Chemical Physics, 1976, 65, 1305-1309.	3.0	36
158	Cryogenic Electron Tunneling within Mixed-Metal Hemoglobin Hybrids:Â Protein Glassing and Electron-Transfer Energetics. Journal of the American Chemical Society, 1998, 120, 11401-11407.	13.7	36
159	â€œSupersaturatedâ€•Self-Assembled Charge-Selective Interfacial Layers for Organic Solar Cells. Journal of the American Chemical Society, 2014, 136, 17762-17773.	13.7	36
160	Piezoresistivity in single DNA molecules. Nature Communications, 2015, 6, 8032.	12.8	36
161	Barrier crossing with concentration boundary conditions in biological channels and chemical reactions. Journal of Chemical Physics, 1993, 98, 1193-1212.	3.0	35
162	Coarse-Grained Molecular Dynamics Study of Cyclic Peptide Nanotube Insertion into a Lipid Bilayer. Journal of Physical Chemistry A, 2009, 113, 4780-4787.	2.5	35

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163	Molecular Donorâ€“Bridgeâ€“Acceptor Strategies for High-Capacitance Organic Dielectric Materials. Journal of the American Chemical Society, 2015, 137, 7189-7196.	13.7	35
164	Hydrogenation of CO to Methanol on Ni(110) through Subsurface Hydrogen. Journal of the American Chemical Society, 2017, 139, 17582-17589.	13.7	35
165	Tunneling Currents That Increase with Molecular Elongation. Journal of the American Chemical Society, 2011, 133, 15714-15720.	13.7	34
166	Polymer fractureâ€”A simple model for chain scission. Journal of Polymer Science, Polymer Physics Edition, 1984, 22, 881-897.	1.0	33
167	Superexchangeâ€Assisted Throughâ€Bridge Electron Transfer: Electronic and Dynamical Aspects. Israel Journal of Chemistry, 1990, 30, 45-58.	2.3	33
168	Catalysis by a Zinc-Porphyrin-Based Metalâ€“Organic Framework: From Theory to Computational Design. Journal of Physical Chemistry C, 2012, 116, 23494-23502.	3.1	33
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