Sergei Tretiak

List of Publications by Year
in descending order

382 papers	28,504 citations	7561 77 h-index	6465 157 g-index
393 all docs	393 docs citations	393 times ranked	24183 citing authors

#	Article	IF	Citations
1	High-efficiency solution-processed perovskite solar cells with millimeter-scale grains. Science, 2015, 347, 522-525.	6.0	2,978
2	High-efficiency two-dimensional Ruddlesdenâ€“Popper perovskite solar cells. Nature, 2016, 536, 312-316.	13.7	2,767
3	Extremely efficient internal exciton dissociation through edge states in layered 2D perovskites. Science, 2017, 355, 1288-1292.	6.0	830
4	Spectrally Resolved Dynamics of Energy Transfer in Quantum-Dot Assemblies: Towards Engineered Energy Flows in Artificial Materials. Physical Review Letters, 2002, 89, 186802.	2.9	617
5	Light-activated photocurrent degradation and self-healing in perovskite solar cells. Nature Communications, 2016, 7, 11574.	5.8	584
6	Scaling law for excitons in 2D perovskite quantum wells. Nature Communications, 2018, 9, 2254.	5.8	559
7	Light-induced lattice expansion leads to high-efficiency perovskite solar cells. Science, 2018, 360, 67-70.	6.0	554
8	Density Matrix Analysis and Simulation of Electronic Excitations in Conjugated and Aggregated Molecules. Chemical Reviews, 2002, 102, 3171-3212.	23.0	519
9	Enhanced Twoâ€Photon Absorption of Organic Chromophores: Theoretical and Experimental Assessments. Advanced Materials, 2008, 20, 4641-4678.	11.1	502
10	Type-II Core/Shell CdS/ZnSe Nanocrystals:â€‰ Synthesis, Electronic Structures, and Spectroscopic Properties. Journal of the American Chemical Society, 2007, 129, 11708-11719.	6.6	402
11	Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. Nature Communications, 2019, 10, 2903.	5.8	399
12	Advances and Promises of Layered Halide Hybrid Perovskite Semiconductors. ACS Nano, 2016, 10, 9776-9786.	7.3	351
13	Electronic Coherence and Collective Optical Excitations of Conjugated Molecules. Science, 1997, 277, 781-787.	6.0	345
14	Effects of (Multi)branching of Dipolar Chromophores on Photophysical Properties and Two-Photon Absorption. Journal of Physical Chemistry A, 2005, 109, 3024-3037.	1.1	341
15	Conformational Dynamics of Photoexcited Conjugated Molecules. Physical Review Letters, 2002, 89, 097402.	2.9	340
16	Dependence of Spurious Charge-Transfer Excited States on Orbital Exchange in TDDFT:â€‰ Large Molecules and Clusters. Journal of Chemical Theory and Computation, 2007, 3, 976-987.	2.3	295
17	Third and Fourth Optical Transitions in Semiconducting Carbon Nanotubes. Physical Review Letters, 2007, 98, 067401.	2.9	274
18	Stable Lightâ€Emitting Diodes Using Phaseâ€Pure Ruddlesdenâ€“Popper Layered Perovskites. Advanced Materials, 2018, 30, 1704217.	11.1	258

#	Article	IF	Citations
19	Effect of Surface Ligands on Optical and Electronic Spectra of Semiconductor Nanoclusters. Journal of the American Chemical Society, 2009, 131, 7717-7726.	6.6	245
20	Polaron Stabilization by Cooperative Lattice Distortion and Cation Rotations in Hybrid Perovskite Materials. Nano Letters, 2016, 16, 3809-3816.	4.5	245
21	Non-adiabatic Excited-State Molecular Dynamics: Theory and Applications for Modeling Photophysics in Extended Molecular Materials. Chemical Reviews, 2020, 120, 2215-2287.	23.0	231
22	Effect of Quantum and Dielectric Confinement on the Excitonâ^'Exciton Interaction Energy in Type II Core/Shell Semiconductor Nanocrystals. Nano Letters, 2007, 7, 108-115.	4.5	217
23	Stilbenoid Dimers:â€‰ Dissection of a Paracyclophane Chromophore. Journal of the American Chemical Society, 1998, 120, 9188-9204.	6.6	214
24	Morphology Effectively Controls Singlet-Triplet Exciton Relaxation and Charge Transport in Organic Semiconductors. Physical Review Letters, 2009, 102, 017401.	2.9	213
25	Nonadiabatic Excited-State Molecular Dynamics: Modeling Photophysics in Organic Conjugated Materials. Accounts of Chemical Research, 2014, 47, 1155-1164.	7.6	201
26	Localized Electronic Excitations in Phenylacetylene Dendrimers. Journal of Physical Chemistry B, 1998, 102, 3310-3315.	1.2	198
27	Critical Role of Interface and Crystallinity on the Performance and Photostability of Perovskite Solar Cell on Nickel Oxide. Advanced Materials, 2018, 30, 1703879.	11.1	198
28	Exciton sizes of conducting polymers predicted by time-dependent density functional theory. Physical Review B, 2005, 71, .	1.1	192
29	Prediction of Two-Photon Absorption Properties for Organic Chromophores Using Time-Dependent Density-Functional Theory. Journal of Physical Chemistry B, 2004, 108, 899-907.	1.2	178
30	Identification of unavoided crossings in nonadiabatic photoexcited dynamics involving multiple electronic states in polyatomic conjugated molecules. Journal of Chemical Physics, 2012, 137, 014512.	1.2	175
31	Real-time observation of nonlinear coherent phonon dynamics in single-walled carbon nanotubes. Nature Physics, 2006, 2, 515-520.	6.5	174
32	Nonadiabatic Excited-State Molecular Dynamics Modeling of Photoinduced Dynamics in Conjugated Molecules. Journal of Physical Chemistry B, 2011, 115, 5402-5414.	1.2	172
33	Light Amplification Using Inverted Core/Shell Nanocrystals:Â Towards Lasing in the Single-Exciton Regime. Journal of Physical Chemistry B, 2004, 108, 10625-10630.	1.2	165
34	Two-Photon Absorption in Three-Dimensional Chromophores Based on [2.2]-Paracyclophane. Journal of the American Chemical Society, 2004, 126, 11529-11542.	6.6	161
35	Light-Driven and Phonon-Assisted Dynamics in Organic and Semiconductor Nanostructures. Chemical Reviews, 2015, 115, 5929-5978.	23.0	160
36	A sensitive and robust thin-film x-ray detector using 2D layered perovskite diodes. Science Advances, 2020, 6, eaay0815.	4.7	153

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37	Composite Nature of Layered Hybrid Perovskites: Assessment on Quantum and Dielectric Confinements and Band Alignment. ACS Nano, 2018, 12, 3321-3332.	7.3	146
38	Resonant nonlinear polarizabilities in the time-dependent density functional theory. Journal of Chemical Physics, 2003, 119, 8809-8823.	1.2	142
39	Self-Trapping of Excitons, Violation of Condon Approximation, and Efficient Fluorescence in Conjugated Cycloparaphenylenes. Nano Letters, 2014, 14, 6539-6546.	4.5	142
40	Scanning Tunneling Microscopy of DNA-Wrapped Carbon Nanotubes. Nano Letters, 2009, 9, 12-17.	4.5	140
41	Electronic Structure and Chemical Nature of Oxygen Dopant States in Carbon Nanotubes. ACS Nano, 2014, 8, 10782-10789.	7.3	131
42	Effect of Precursor Solution Aging on the Crystallinity and Photovoltaic Performance of Perovskite Solar Cells. Advanced Energy Materials, 2017, 7, 1602159.	10.2	130
43	Excited-state vibrational dynamics toward the polaron in methylammonium lead iodide perovskite. Nature Communications, 2018, 9, 2525.	5.8	129
44	Surface Ligands Increase Photoexcitation Relaxation Rates in CdSe Quantum Dots. ACS Nano, 2012, 6, 6515-6524.	7.3	128
45	Bacteriochlorophyll and Carotenoid Excitonic Couplings in the LH2 System of Purple Bacteria. Journal of Physical Chemistry B, 2000, 104, 9540-9553.	1.2	127
46	Two-Photon Transitions in Quadrupolar and Branched Chromophores:â€‰ Experiment and Theory. Journal of Physical Chemistry B, 2007, 111, 9468-9483.	1.2	127
47	Nonadiabatic excited-state molecular dynamics: Treatment of electronic decoherence. Journal of Chemical Physics, 2013, 138, 224111.	1.2	127
48	Two-Dimensional Real-Space Analysis of Optical Excitations in Acceptor-Substituted Carotenoids. Journal of the American Chemical Society, 1997, 119, 11408-11419.	6.6	123
49	Passivating ligand and solvent contributions to the electronic properties of semiconductor nanocrystals. Nanoscale, 2012, 4, 904-914.	2.8	123
50	Femtosecond torsional relaxation. Nature Physics, 2012, 8, 225-231.	6.5	122
51	Energetic Chromophores: Low-Energy Laser Initiation in Explosive Fe(II) Tetrazine Complexes. Journal of the American Chemical Society, 2016, 138, 4685-4692.	6.6	120
52	Oligophenylenevinylene Phane Dimers:Â Probing the Effect of Contact Site on the Optical Properties of Bichromophoric Pairs. Journal of the American Chemical Society, 2000, 122, 1289-1297.	6.6	116
53	Exciton Hamiltonian for the Bacteriochlorophyll System in the LH2 Antenna Complex of Purple Bacteria. Journal of Physical Chemistry B, 2000, 104, 4519-4528.	1.2	114
54	Polarons in Halide Perovskites: A Perspective. Journal of Physical Chemistry Letters, 2020, 11, 3271-3286.	2.1	110

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55	Electron-Vibrational Dynamics of Photoexcited Polyfluorenes. Journal of the American Chemical Society, 2004, 126, 12130-12140.	6.6	108
56	Computational Dissection of Two-Dimensional Rectangular Titanium Mononitride TiN: Auxetics and Promises for Photocatalysis. Nano Letters, 2017, 17, 4466-4472.	4.5	104
57	The ANI-1ccx and ANI-1x data sets, coupled-cluster and density functional theory properties for molecules. Scientific Data, 2020, 7, 134.	2.4	104
58	Concept of Lattice Mismatch and Emergence of Surface States in Two-dimensional Hybrid Perovskite Quantum Wells. Nano Letters, 2018, 18, 5603-5609.	4.5	103
59	Localization of Electronic Excitations in Conjugated Polymers Studied by DFT. Journal of Physical Chemistry Letters, 2011, 2, 566-571.	2.1	96
60	Excitonic couplings and electronic coherence in bridged naphthalene dimers. Proceedings of the National Academy of Sciences of the United States of America, 1999, 96, 13003-13008.	3.3	95
61	Reaction Dynamics of a Photochromic Fluorescing Dithienylethene. Journal of Physical Chemistry A, 2001, 105, 1741-1749.	1.1	93
62	Absorption cross sections and Auger recombination lifetimes in inverted core-shell nanocrystals: Implications for lasing performance. Journal of Applied Physics, 2006, 99, 034309.	1.1	93
63	Representation independent algorithms for molecular response calculations in time-dependent self-consistent field theories. Journal of Chemical Physics, 2009, 130, 054111.	1.2	92
64	Size Scaling of Third-Order Off-Resonant Polarizabilities. Electronic Coherence in Organic Oligomers. Journal of the American Chemical Society, 2000, 122, 452-459.	6.6	91
65	Exciton scattering and localization in branched dendrimeric structures. Nature Physics, 2006, 2, 631-635.	6.5	91
66	Exciton-scaling and optical excitations of self-similar phenylacetylene dendrimers. Journal of Chemical Physics, 1999, 110, 8161-8175.	1.2	90
67	How Chromophore Shape Determines the Spectroscopy of Phenyleneâ^'Vinylenes:â€‰ Origin of Spectral Broadening in the Absence of Aggregation. Journal of Physical Chemistry B, 2008, 112, 4859-4864.	1.2	90
68	Reaction dynamics of photochromic dithienylethene derivatives. Chemical Physics, 1999, 246, 115-125.	0.9	89
69	A new pH sensitive fluorescent and white light emissive material through controlled intermolecular charge transfer. Chemical Science, 2015, 6, 789-797.	3.7	89
70	Discovering a Transferable Charge Assignment Model Using Machine Learning. Journal of Physical Chemistry Letters, 2018, 9, 4495-4501.	2.1	88
71	Interchain Electronic Excitations in Poly(phenylenevinylene) (PPV) Aggregates. Journal of Physical Chemistry B, 2000, 104, 7029-7037.	1.2	85
72	Nonadiabatic excited-state molecular dynamics: Numerical tests of convergence and parameters. Journal of Chemical Physics, 2012, 136, 054108.	1.2	84

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73	Theoretical Description of Structural and Electronic Properties of Organic Photovoltaic Materials. Annual Review of Physical Chemistry, 2015, 66, 305-330.	4.8	82
74	Analysis of Absorption Spectra of Zinc Porphyrin, Zinc meso-Tetraphenylporphyrin, and Halogenated Derivatives. Journal of Physical Chemistry A, 2002, 106, 10285-10293.	1.1	81
75	Transferable Dynamic Molecular Charge Assignment Using Deep Neural Networks. Journal of Chemical Theory and Computation, 2018, 14, 4687-4698.	2.3	81
76	Collective electronic oscillators for nonlinear optical response of conjugated molecules. Chemical Physics Letters, 1996, 259, 55-61.	1.2	80
77	Triplet State Absorption in Carbon Nanotubes:Â A TDâ˜DFT Study. Nano Letters, 2007, 7, 2201-2206.	4.5	80
78	Electronic Structure of Ligated CdSe Clusters: Dependence on DFT Methodology. Journal of Physical Chemistry C, 2011, 115, 15793-15800.	1.5	80
79	Krylov-space algorithms for time-dependent Hartreeâ€“Fock and density functional computations. Journal of Chemical Physics, 2000, 113, 36-43.	1.2	79
80	Low-Temperature Single Carbon Nanotube Spectroscopy of sp³ Quantum Defects. ACS Nano, 2017, 11, 10785-10796.	7.3	79
81	Narrow-band single-photon emission through selective aryl functionalization of zigzag carbon nanotubes. Nature Chemistry, 2018, 10, 1089-1095.	6.6	78
82	Nonadiabatic Molecular Dynamics Simulations of the Energy Transfer between Building Blocks in a Phenylene Ethynylene Dendrimer. Journal of Physical Chemistry A, 2009, 113, 7535-7542.	1.1	76
83	Plasmonic Hot-Carrier-Mediated Tunable Photochemical Reactions. ACS Nano, 2018, 12, 8415-8422.	7.3	75
84	Recursive densityâ€matrixâ€spectralâ€moment algorithm for molecular nonlinear polarizabilities. Journal of Chemical Physics, 1996, 105, 8914-8928.	1.2	72
85	Brightening of the Lowest Exciton in Carbon Nanotubes via Chemical Functionalization. Nano Letters, 2012, 12, 2306-2312.	4.5	72
86	Structurally Defined 3D Nanographene Assemblies via Bottomâ€Up Chemical Synthesis for Highly Efficient Lithium Storage. Advanced Materials, 2016, 28, 10250-10256.	11.1	72
87	Charge carrier dynamics in two-dimensional hybrid perovskites: Dionâ€“Jacobson vs. Ruddlesdenâ€“Popper phases. Journal of Materials Chemistry A, 2020, 8, 22009-22022.	5.2	72
88	Coherent exciton-vibrational dynamics and energy transfer in conjugated organics. Nature Communications, 2018, 9, 2316.	5.8	71
89	Photoexcited breathers in conjugated polyenes: An excited-state molecular dynamics study. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 2185-2190.	3.3	68
90	A joint theoretical and experimental study of phenyleneâ€“acetylene molecular wires. Chemical Physics Letters, 2005, 401, 149-156.	1.2	68

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91	Comparison of TD-DFT Methods for the Calculation of Two-Photon Absorption Spectra of Oligophenylvinylenes. Journal of Physical Chemistry C, 2013, 117, 18170-18189.	1.5	68
92	Fluorescent Carbon Nanotube Defects Manifest Substantial Vibrational Reorganization. Journal of Physical Chemistry C, 2016, 120, 11268-11276.	1.5	68
93	Simulations of two-dimensional femtosecond infrared photon echoes of glycine dipeptide. Journal of Raman Spectroscopy, 2000, 31, 125-135.	1.2	67
94	Electronic Structure of Self-Assembled Amorphous Polyfluorenes. ACS Nano, 2008, 2, 1381-1388.	7.3	65
95	The Effects of Electronic Impurities and Electronâ€“Hole Recombination Dynamics on Largeâ€Grain Organicâ€“Inorganic Perovskite Photovoltaic Efficiencies. Advanced Functional Materials, 2016, 26, 4283-4292.	7.8	65
96	DFT Study of Ligand Binding to Small Gold Clusters. Journal of Physical Chemistry Letters, 2010, 1, 927-931.	2.1	64
97	Chemical Bonding and Size Scaling of Nonlinear Polarizabilities of Conjugated Polymers. Physical Review Letters, 1996, 77, 4656-4659.	2.9	62
98	Excitonic effects in a time-dependent density functional theory. Journal of Chemical Physics, 2007, 127, 114902.	1.2	61
99	Determination of Exciton-Phonon Coupling Elements in Single-Walled Carbon Nanotubes by Raman Overtone Analysis. Physical Review Letters, 2007, 98, 037405.	2.9	61
100	Lattice Expansion in Hybrid Perovskites: Effect on Optoelectronic Properties and Charge Carrier Dynamics. Journal of Physical Chemistry Letters, 2019, 10, 5000-5007.	2.1	60
101	Theoretical study of the effects of solvent environment on photophysical properties and electronic structure of paracyclophane chromophores. Journal of Chemical Physics, 2005, 122, 224505.	1.2	59
102	Excitonic and Vibrational Properties of Singleâ€Walled Semiconducting Carbon Nanotubes. Advanced Functional Materials, 2007, 17, 3405-3420.	7.8	59
103	Unidirectional Energy Transfer in Conjugated Molecules: The Crucial Role of High-Frequency Câ‰¡C Bonds. Journal of Physical Chemistry Letters, 2010, 1, 2699-2704.	2.1	59
104	Ligands Slow Down Pure-Dephasing in Semiconductor Quantum Dots. ACS Nano, 2015, 9, 9106-9116.	7.3	59
105	Electronic Delocalization, Vibrational Dynamics, and Energy Transfer in Organic Chromophores. Journal of Physical Chemistry Letters, 2017, 8, 3020-3031.	2.1	59
106	Quantum chemistry of the minimal CdSe clusters. Journal of Chemical Physics, 2008, 129, 074709.	1.2	58
107	Non-radiative relaxation of photoexcited chlorophylls: theoretical and experimental study. Scientific Reports, 2015, 5, 13625.	1.6	58
108	Exciton Localization and Optical Emission in Aryl-Functionalized Carbon Nanotubes. Journal of Physical Chemistry C, 2018, 122, 1828-1838.	1.5	58

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109	A Combined Experimental and Theoretical Study of Conformational Preferences of Molecular Semiconductors. Journal of Physical Chemistry C, 2014, 118, 15610-15623.	1.5	57
110	Electronic Properties of DNA Base Molecules Adsorbed on a Metallic Surface. Journal of Physical Chemistry C, 2007, 111, 14541-14551.	1.5	56
111	Ideal dipole approximation fails to predict electronic coupling and energy transfer between semiconducting single-wall carbon nanotubes. Journal of Chemical Physics, 2009, 130, 081104.	1.2	56
112	Effect of deprotonation on absorption and emission spectra of Ru(ii)-bpy complexes functionalized with carboxyl groups. Physical Chemistry Chemical Physics, 2010, 12, 8902.	1.3	56
113	Shishiodoshi unidirectional energy transfer mechanism in phenylene ethynylene dendrimers. Journal of Chemical Physics, 2012, 137, 22A526.	1.2	56
114	Photoluminescence imaging of solitary dopant sites in covalently doped single-wall carbon nanotubes. Nanoscale, 2015, 7, 20521-20530.	2.8	56
115	NEXMD Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 5771-5783.	2.3	56
116	Role of Donorâ^'Acceptor Strengths and Separation on the Two-Photon Absorption Response of Cytotoxic Dyes:â€‰ A TD-DFT Study. Journal of Physical Chemistry A, 2005, 109, 7276-7284.	1.1	55
117	Comparison of LC-TDDFT and ADC(2) Methods in Computations of Bright and Charge Transfer States in Stacked Oligothiophenes. Journal of Chemical Theory and Computation, 2014, 10, 3280-3289.	2.3	54
118	First-Principles Study of p-n-Doped Silicon Quantum Dots: Charge Transfer, Energy Dissipation, and Time-Resolved Emission. Journal of Physical Chemistry Letters, 2013, 4, 2906-2913.	2.1	53
119	Artifacts due to trivial unavoided crossings in the modeling of photoinduced energy transfer dynamics in extended conjugated molecules. Chemical Physics Letters, 2013, 590, 208-213.	1.2	53
120	Simultaneous Control of Emission Localization and Two-Photon Absorption Efficiency in Dissymmetrical Chromophores. Journal of Physical Chemistry B, 2010, 114, 3152-3169.	1.2	52
121	Geometry Distortion and Small Polaron Binding Energy Changes with Ionic Substitution in Halide Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 7130-7136.	2.1	52
122	Controlling Defect-State Photophysics in Covalently Functionalized Single-Walled Carbon Nanotubes. Accounts of Chemical Research, 2020, 53, 1791-1801.	7.6	52
123	Violation of the Condon Approximation in Semiconducting Carbon Nanotubes. ACS Nano, 2011, 5, 5233-5241.	7.3	51
124	Non-adiabatic excited state molecular dynamics of phenylene ethynylene dendrimer using a multiconfigurational Ehrenfest approach. Physical Chemistry Chemical Physics, 2016, 18, 10028-10040.	1.3	51
125	Analysis of State-Specific Vibrations Coupled to the Unidirectional Energy Transfer in Conjugated Dendrimers. Journal of Physical Chemistry A, 2012, 116, 9802-9810.	1.1	50
126	Role of Geometric Distortion and Polarization in Localizing Electronic Excitations in Conjugated Polymers. Journal of Chemical Theory and Computation, 2013, 9, 1144-1154.	2.3	50

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127	Dynamics of Energy Transfer in a Conjugated Dendrimer Driven by Ultrafast Localization of Excitations. Journal of the American Chemical Society, 2015, 137, 11637-11644.	6.6	50
128	Optoelectronic Properties of Two-Dimensional Bromide Perovskites: Influences of Spacer Cations. Journal of Physical Chemistry Letters, 2020, 11, 2955-2964.	2.1	50
129	Cross-polarized excitons in carbon nanotubes. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 6797-6802.	3.3	49
130	Interlayer-Decoupled Sc-Based Mxene with High Carrier Mobility and Strong Light-Harvesting Ability. Journal of Physical Chemistry Letters, 2018, 9, 6915-6920.	2.1	49
131	Excited state molecular dynamics simulations of nonlinear pushâ€“pull chromophores. Chemical Physics Letters, 2003, 367, 293-307.	1.2	47
132	Linear optical response of current-carrying molecular junction: A nonequilibrium Greenâ€™s functionâ€“time-dependent density functional theory approach. Journal of Chemical Physics, 2008, 128, 124705.	1.2	47
133	Ab Initio Study of a Molecular Crystal for Photovoltaics: Light Absorption, Exciton and Charge Carrier Transport. Journal of Physical Chemistry C, 2013, 117, 4920-4930.	1.5	47
134	Automated discovery of a robust interatomic potential for aluminum. Nature Communications, 2021, 12, 1257.	5.8	47
135	Excitons and Peierls Distortion in Conjugated Carbon Nanotubes. Nano Letters, 2007, 7, 86-92.	4.5	46
136	Ultrafast intersystem-crossing in platinum containing Ï€-conjugated polymers with tunable spin-orbit coupling. Scientific Reports, 2013, 3, 2653.	1.6	46
137	Topological Considerations for the Design of Molecular Donors with Multiple Absorbing Units. Journal of the American Chemical Society, 2014, 136, 5591-5594.	6.6	46
138	Solvent effects in time-dependent self-consistent field methods. II. Variational formulations and analytical gradients. Journal of Chemical Physics, 2015, 143, 054305.	1.2	46
139	Effects of Chlorine Mixing on Optoelectronics, Ion Migration, and Gamma-Ray Detection in Bromide Perovskites. Chemistry of Materials, 2020, 32, 1854-1863.	3.2	46
140	Teaching a neural network to attach and detach electrons from molecules. Nature Communications, 2021, 12, 4870.	5.8	46
141	Low-Lying Exciton States Determine the Photophysics of Semiconducting Single Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2007, 111, 11139-11149.	1.5	45
142	Semiclassical Monte-Carlo approach for modelling non-adiabatic dynamics in extended molecules. Nature Communications, 2013, 4, 2144.	5.8	45
143	Two-Photon Excitation of Substituted Enediynes. Journal of Physical Chemistry A, 2006, 110, 241-251.	1.1	44
144	Spectrally resolved hyperfine interactions between polaron and nuclear spins in organic light emitting diodes: Magneto-electroluminescence studies. Applied Physics Letters, 2014, 105, .	1.5	43

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145	Origin, scaling, and saturation of second order polarizabilities in donor/acceptor polyenes. Chemical Physics Letters, 1998, 287, 75-82.	1.2	42
146	Excited states and optical response of a donorâ€“acceptor substituted polyene: A TD-DFT study. Chemical Physics Letters, 2007, 433, 305-311.	1.2	42
147	Formation of Assemblies Comprising Ruâ€“Polypyridine Complexes and CdSe Nanocrystals Studied by ATR-FTIR Spectroscopy and DFT Modeling. Langmuir, 2011, 27, 8377-8383.	1.6	42
148	Electronic structure and optical spectra of semiconducting carbon nanotubes functionalized by diazonium salts. Chemical Physics, 2013, 413, 89-101.	0.9	42
149	Frenkel-exciton Hamiltonian for dendrimeric nanostar. Journal of Luminescence, 2000, 87-89, 115-118.	1.5	41
150	Interâ€Aromatic Distances in Geobacter Sulfurreducens Pili Relevant to Biofilm Charge Transport. Advanced Materials, 2015, 27, 1908-1911.	11.1	41
151	Solvent- and Wavelength-Dependent Photoluminescence Relaxation Dynamics of Carbon Nanotube sp³ Defect States. ACS Nano, 2018, 12, 8060-8070.	7.3	41
152	Tuning Electronic Structure in Layered Hybrid Perovskites with Organic Spacer Substitution. Nano Letters, 2019, 19, 8732-8740.	4.5	41
153	Bright and dark excitons in semiconductor carbon nanotubes: insights from electronic structure calculations. Physical Chemistry Chemical Physics, 2009, 11, 4113.	1.3	40
154	Ultrafast Photodissociation Dynamics of Nitromethane. Journal of Physical Chemistry A, 2016, 120, 519-526.	1.1	39
155	Photoexcited Nonadiabatic Dynamics of Solvated Pushâ€“Pull Ï€-Conjugated Oligomers with the NEXMD Software. Journal of Chemical Theory and Computation, 2018, 14, 3955-3966.	2.3	39
156	Critical Role of Organic Spacers for Bright 2D Layered Perovskites Lightâ€Emitting Diodes. Advanced Science, 2020, 7, 1903202.	5.6	39
157	The Rise of Neural Networks for Materials and Chemical Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 6227-6243.	2.1	39
158	Excitation transfer processes in a phosphor-doped poly(p-phenylene vinylene) light-emitting diode. Physical Review B, 2002, 65, .	1.1	38
159	Calculations of the third-order nonlinear optical responses in pushâ€“pull chromophores with a time-dependent density functional theory. Chemical Physics Letters, 2004, 392, 444-451.	1.2	38
160	Tailored Electronic Structure and Optical Properties of Conjugated Systems through Aggregates and Dipoleâ€“Dipole Interactions. ACS Applied Materials & Interfaces, 2013, 5, 4685-4695.	4.0	38
161	Excited-State Structure of Oligothiophene Dendrimers: Computational and Experimental Study. Journal of Physical Chemistry B, 2010, 114, 15808-15817.	1.2	37
162	Mechanism of Electrolyte-Induced Brightening in Single-Wall Carbon Nanotubes. Journal of the American Chemical Society, 2013, 135, 3379-3382.	6.6	37

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163	Electron-vibrational relaxation of photoexcited polyfluorenes in the presence of chemical defects: A theoretical study. Chemical Physics Letters, 2003, 372, 403-408.	1.2	35
164	Influence of Surfactants and Charges on CdSe Quantum Dots. Journal of Cluster Science, 2011, 22, 405-431.	1.7	35
165	Two-Photon Absorption in CdSe Colloidal Quantum Dots Compared to Organic Molecules. ACS Nano, 2014, 8, 12572-12586.	7.3	35
166	Photoactive High Explosives: Linear and Nonlinear Photochemistry of Petrin Tetrazine Chloride. Journal of Physical Chemistry A, 2015, 119, 4846-4855.	1.1	34
167	Two-dimensional hexagonal M₃C₂ (M = Zn, Cd and Hg) monolayers: novel quantum spin Hall insulators and Dirac cone materials. Journal of Materials Chemistry C, 2017, 5, 9181-9187.	2.7	34
168	Conformational disorder in energy transfer: beyond FÃ¶rster theory. Physical Chemistry Chemical Physics, 2013, 15, 9245.	1.3	33
169	Cation Alloying Delocalizes Polarons in Lead Halide Perovskites. Journal of Physical Chemistry Letters, 2019, 10, 3516-3524.	2.1	33
170	Optical Effects of Divalent Functionalization of Carbon Nanotubes. Chemistry of Materials, 2019, 31, 6950-6961.	3.2	33
171	Excited electronic states of carotenoids: Time-dependent density-matrix-response algorithm. International Journal of Quantum Chemistry, 1998, 70, 711-727.	1.0	32
172	Two-exciton states and spectroscopy of phenylacetylene dendrimers. Journal of Chemical Physics, 1999, 111, 4158-4168.	1.2	32
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