Sergei Tretiak

List of Publications by Year
in descending order

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382 papers	28,504 citations	7568 77 h-index	6471 157 g-index
393 all docs	393 docs citations	393 times ranked	24183 citing authors

#	Article	IF	Citations
1	Nature of electronic excitations in small non-stoichiometric quantum dots. Journal of Materials Chemistry A, 2022, 10, 5212-5220.	10.3	10
2	Vibronic Photoexcitation Dynamics of Perylene Diimide: Computational Insights. Journal of Physical Chemistry A, 2022, 126, 733-741.	2.5	1
3	Induced Chirality in Halide Perovskite Clusters through Surface Chemistry. Journal of Physical Chemistry Letters, 2022, 13, 686-693.	4.6	12
4	Long carrier diffusion length in two-dimensional lead halide perovskite single crystals. CheM, 2022, 8, 1107-1120.	11.7	29
5	Sampling electronic structure quadratic unconstrained binary optimization problems (QUBOs) with Ocean and Mukai solvers. PLoS ONE, 2022, 17, e0263849.	2.5	5
6	Plasmon-Enhanced Exciton Delocalization in Squaraine-Type Molecular Aggregates. ACS Nano, 2022, 16, 4693-4704.	14.6	6
7	Ultrafast coherent photoexcited dynamics in a trimeric dendrimer probed by X-ray stimulated-Raman signals. Chemical Science, 2022, 13, 6373-6384.	7.4	5
8	Control of Polaronic Behavior and Carrier Lifetimes via Metal and Anion Alloying in Chalcogenide Perovskites. Journal of Physical Chemistry Letters, 2022, 13, 4955-4962.	4.6	7
9	Toward a QUBO-Based Density Matrix Electronic Structure Method. Journal of Chemical Theory and Computation, 2022, 18, 4177-4185.	5.3	2
10	Point Defects in Two-Dimensional Ruddlesdenâ€“Popper Perovskites Explored with Ab Initio Calculations. Journal of Physical Chemistry Letters, 2022, 13, 5213-5219.	4.6	11
11	Impact of Graphene Quantum Dot Edge Morphologies on Their Optical Properties. Journal of Physical Chemistry Letters, 2022, 13, 5801-5807.	4.6	5
12	Two Dimensional MOene: From Superconductors to Direct Semiconductors and Weyl Fermions. Nano Letters, 2022, 22, 5592-5599.	9.1	8
13	Deep learning of dynamically responsive chemical Hamiltonians with semiempirical quantum mechanics. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	19
14	(Invited) Theoretical Insight into New Strategies of Carbon Nanotube Functionalization. ECS Meeting Abstracts, 2022, MA2022-01, 738-738.	0.0	0
15	Intermolecular conical intersections in molecular aggregates. Nature Nanotechnology, 2021, 16, 63-68.	31.5	22
16	Exciton Spatial Dynamics and Self-Trapping in Carbon Nanocages. Journal of Physical Chemistry Letters, 2021, 12, 224-231.	4.6	3
17	Monitoring molecular vibronic coherences in a bichromophoric molecule by ultrafast X-ray spectroscopy. Chemical Science, 2021, 12, 5286-5294.	7.4	16
18	Highly efficient photoelectric effect in halide perovskites for regenerative electron sources. Nature Communications, 2021, 12, 673.	12.8	13

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19	Automated discovery of a robust interatomic potential for aluminum. Nature Communications, 2021, 12, 1257.	12.8	47
20	Interplay between Electrostatic Properties of Molecular Adducts and Their Positions at Carbon Nanotubes. Journal of Physical Chemistry C, 2021, 125, 4785-4793.	3.1	10
21	Reduction of the molecular hamiltonian matrix using quantum community detection. Scientific Reports, 2021, 11, 4099.	3.3	11
22	Nonadiabatic Excited-State Molecular Dynamics Methodologies: Comparison and Convergence. Journal of Physical Chemistry Letters, 2021, 12, 2970-2982.	4.6	20
23	Tunable Optical Features of Graphene Quantum Dots from Edge Functionalization. Journal of Physical Chemistry C, 2021, 125, 9244-9252.	3.1	23
24	Millimeterâ€Size Allâ€inorganic Perovskite Crystalline Thin Film Grown by Chemical Vapor Deposition. Advanced Functional Materials, 2021, 31, 2101058.	14.9	19
25	Enantioselectivity in the Noyoriâ€“Ikariya Asymmetric Transfer Hydrogenation of Ketones. Organometallics, 2021, 40, 1402-1410.	2.3	24
26	An Ab Initio Multiple Cloning Method for Non-Adiabatic Excited-State Molecular Dynamics in NWChem. Journal of Chemical Theory and Computation, 2021, 17, 3629-3643.	5.3	15
27	(Invited) Theoretical Insights into New Strategies of Carbon Nanotube Functionalization. ECS Meeting Abstracts, 2021, MA2021-01, 575-575.	0.0	0
28	Nonadiabatic Molecular Dynamics Study of the Relaxation Pathways of Photoexcited Cyclooctatetraene. Journal of Physical Chemistry Letters, 2021, 12, 5716-5722.	4.6	5
29	Photoinduced Energy Transfer in Linear Guestâ€“Host Chromophores: A Computational Study. Journal of Physical Chemistry A, 2021, 125, 5303-5313.	2.5	5
30	Machine learned HÃ¼ckel theory: Interfacing physics and deep neural networks. Journal of Chemical Physics, 2021, 154, 244108.	3.0	25
31	Cesium-Coated Halide Perovskites as a Photocathode Material: Modeling Insights. Journal of Physical Chemistry Letters, 2021, 12, 6269-6276.	4.6	7
32	The Rise of Neural Networks for Materials and Chemical Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 6227-6243.	4.6	39
33	Coupling between Emissive Defects on Carbon Nanotubes: Modeling Insights. Journal of Physical Chemistry Letters, 2021, 12, 7846-7853.	4.6	10
34	Hot Carrier Dynamics at Ligated Silicon(111) Surfaces: A Computational Study. Journal of Physical Chemistry Letters, 2021, 12, 7504-7511.	4.6	3
35	Teaching a neural network to attach and detach electrons from molecules. Nature Communications, 2021, 12, 4870.	12.8	46
36	Robust Unencapsulated Perovskite Solar Cells Protected by a Fluorinated Fullerene Electron Transporting Layer. ACS Energy Letters, 2021, 6, 3376-3385.	17.4	27

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37	Computing molecular excited states on a D-Wave quantum annealer. Scientific Reports, 2021, 11, 18796.	3.3	16
38	Enhanced Emission from Bright Excitons in Asymmetrically Strained Colloidal CdSe/Cd_xZn_{1â€“x}Se Quantum Dots. ACS Nano, 2021, 15, 14444-14452.	14.6	9
39	Excitation Energy Transfer between bodipy Dyes in a Symmetric Molecular Excitonic Seesaw. Journal of Physical Chemistry A, 2021, 125, 8404-8416.	2.5	2
40	Photoluminescence Dynamics Defined by Exciton Trapping Potential of Coupled Defect States in DNA-Functionalized Carbon Nanotubes. ACS Nano, 2021, 15, 923-933.	14.6	15
41	Predicting phosphorescence energies and inferring wavefunction localization with machine learning. Chemical Science, 2021, 12, 10207-10217.	7.4	14
42	Excited-State Properties of Defected Halide Perovskite Quantum Dots: Insights from Computation. Journal of Physical Chemistry Letters, 2021, 12, 1005-1011.	4.6	15
43	Microcrystal Electron Diffraction for Molecular Design of Functional Non-Fullerene Acceptor Structures. Chemistry of Materials, 2021, 33, 966-977.	6.7	12
44	Structural Dynamics and Electronic Properties of Semiconductor Quantum Dots: Computational Insights. Chemistry of Materials, 2021, 33, 7848-7857.	6.7	14
45	Back-and-Forth Energy Transfer during Electronic Relaxation in a Chlorinâ€“Perylene Dyad. Journal of Physical Chemistry Letters, 2021, 12, 10394-10401.	4.6	1
46	Single-Layer Dititanium Oxide Ti₂O MOene: Multifunctional Promises for Electride, Anode Materials, and Superconductor. Journal of Physical Chemistry Letters, 2021, 12, 494-500.	4.6	12
47	Nonadiabatic molecular dynamics analysis of hybrid Dionâ€“Jacobson 2D leads iodide perovskites. Applied Physics Letters, 2021, 119, .	3.3	9
48	Frenkel biexcitons in hybrid HJ photophysical aggregates. Science Advances, 2021, 7, eabi5197.	10.3	10
49	Recent advances of novel ultrathin two-dimensional silicon carbides from a theoretical perspective. Nanoscale, 2020, 12, 4269-4282.	5.6	31
50	Importance of Vacancies and Doping in the Hole-Transporting Nickel Oxide Interface with Halide Perovskites. ACS Applied Materials & Interfaces, 2020, 12, 6633-6640.	8.0	21
51	Photoinduced Dynamics with Constrained Vibrational Motion: FrozeNM Algorithm. Journal of Chemical Theory and Computation, 2020, 16, 7289-7298.	5.3	7
52	Vibrational energy redistribution during donorâ€“acceptor electronic energy transfer: criteria to identify subsets of active normal modes. Physical Chemistry Chemical Physics, 2020, 22, 18454-18466.	2.8	14
53	An extended moments model of quantum efficiency for metals and semiconductors. Journal of Applied Physics, 2020, 128, .	2.5	6
54	Passivating Nucleobases Bring Charge Transfer Character to Optically Active Transitions in Small Silver Nanoclusters. Journal of Physical Chemistry A, 2020, 124, 8931-8942.	2.5	3

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55	Charge carrier dynamics in two-dimensional hybrid perovskites: Dionâ€“Jacobson vs. Ruddlesdenâ€“Popper phases. Journal of Materials Chemistry A, 2020, 8, 22009-22022.	10.3	72
56	Role of the Metalâ€“Semiconductor Interface in Halide Perovskite Devices for Radiation Photon Counting. ACS Applied Materials & Interfaces, 2020, 12, 45533-45540.	8.0	21
57	Hot Carrier Cooling and Recombination Dynamics of Chlorine-Doped Hybrid Perovskite Single Crystals. Journal of Physical Chemistry Letters, 2020, 11, 8430-8436.	4.6	11
58	Machine learning approaches for structural and thermodynamic properties of a Lennard-Jones fluid. Journal of Chemical Physics, 2020, 153, 104502.	3.0	22
59	Controlling Defect-State Photophysics in Covalently Functionalized Single-Walled Carbon Nanotubes. Accounts of Chemical Research, 2020, 53, 1791-1801.	15.6	52
60	First Principles Nonadiabatic Excited-State Molecular Dynamics in NWChem. Journal of Chemical Theory and Computation, 2020, 16, 6418-6427.	5.3	20
61	Electronic structure with direct diagonalization on a D-wave quantum annealer. Scientific Reports, 2020, 10, 20753.	3.3	18
62	The ANI-1ccx and ANI-1x data sets, coupled-cluster and density functional theory properties for molecules. Scientific Data, 2020, 7, 134.	5.3	104
63	Electronic Energy Relaxation in a Photoexcited Fully Fused Edge-Sharing Carbon Nanobelt. Journal of Physical Chemistry Letters, 2020, 11, 4711-4719.	4.6	8
64	Ex Machina Determination of Structural Correlation Functions. Journal of Physical Chemistry Letters, 2020, 11, 4372-4378.	4.6	7
65	Correlation of Spatiotemporal Dynamics of Polarization and Charge Transport in Blended Hybrid Organicâ€“Inorganic Perovskites on Macro- and Nanoscales. ACS Applied Materials & Interfaces, 2020, 12, 15380-15388.	8.0	5
66	Nonadiabatic Excited-State Molecular Dynamics for Open-Shell Systems. Journal of Chemical Theory and Computation, 2020, 16, 2053-2064.	5.3	10
67	Optoelectronic Properties of Two-Dimensional Bromide Perovskites: Influences of Spacer Cations. Journal of Physical Chemistry Letters, 2020, 11, 2955-2964.	4.6	50
68	Polarons in Halide Perovskites: A Perspective. Journal of Physical Chemistry Letters, 2020, 11, 3271-3286.	4.6	110
69	Methylammonium Lead Tribromide Single Crystal Detectors towards Robust Gammaâ€Ray Photon Sensing. Advanced Optical Materials, 2020, 8, 2000233.	7.3	18
70	Photoexcited energy relaxation and vibronic couplings in Ï€-conjugated carbon nanorings. Physical Chemistry Chemical Physics, 2020, 22, 15321-15332.	2.8	4
71	Graphics Processing Unit-Accelerated Semiempirical Born Oppenheimer Molecular Dynamics Using PyTorch. Journal of Chemical Theory and Computation, 2020, 16, 4951-4962.	5.3	24
72	NEXMD Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 5771-5783.	5.3	56

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73	Analytic model of electron transport through and over non-linear barriers. Journal of Applied Physics, 2020, 127, 235301.	2.5	16
74	Non-adiabatic Excited-State Molecular Dynamics: Theory and Applications for Modeling Photophysics in Extended Molecular Materials. Chemical Reviews, 2020, 120, 2215-2287.	47.7	231
75	Critical Role of Organic Spacers for Bright 2D Layered Perovskites Lightâ€Emitting Diodes. Advanced Science, 2020, 7, 1903202.	11.2	39
76	Multifunctional Cellulose Nanocrystals as a High-Efficient Polysulfide Stopper for Practical Liâ€“S Batteries. ACS Applied Materials & Interfaces, 2020, 12, 17592-17601.	8.0	22
77	Hidden Fine Structure of Quantum Defects Revealed by Single Carbon Nanotube Magneto-Photoluminescence. ACS Nano, 2020, 14, 3451-3460.	14.6	14
78	Effects of Chlorine Mixing on Optoelectronics, Ion Migration, and Gamma-Ray Detection in Bromide Perovskites. Chemistry of Materials, 2020, 32, 1854-1863.	6.7	46
79	The working principle of hybrid perovskite gamma-ray photon counter. Materials Today, 2020, 37, 27-34.	14.2	22
80	A sensitive and robust thin-film x-ray detector using 2D layered perovskite diodes. Science Advances, 2020, 6, eaay0815.	10.3	153
81	Vibronic Quantum Beating between Electronic Excited States in a Heterodimer. Journal of Physical Chemistry B, 2020, 124, 3992-4001.	2.6	12
82	Experimental and theoretical study of energy transfer in a chromophore triad: What makes modeling dynamics successful?. Journal of Chemical Physics, 2020, 153, 244114.	3.0	8
83	Photoexcitation dynamics in perylene diimide dimers. Journal of Chemical Physics, 2020, 153, 244117.	3.0	8
84	(Invited) Controlling Defect-State Emission in Covalently Functionalized Single-Walled Carbon Nanotubes: A Theoretical Perspective. ECS Meeting Abstracts, 2020, MA2020-01, 692-692.	0.0	0
85	Ultrafast nonadiabatic dynamics through an intermolecular conical intersection. , 2020, , .		0
86	Lattice Expansion in Hybrid Perovskites: Effect on Optoelectronic Properties and Charge Carrier Dynamics. Journal of Physical Chemistry Letters, 2019, 10, 5000-5007.	4.6	60
87	Tuning Optical Properties of Conjugated Molecules by Lewis Acids: Insights from Electronic Structure Modeling. Journal of Physical Chemistry Letters, 2019, 10, 4632-4638.	4.6	14
88	Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. Nature Communications, 2019, 10, 2903.	12.8	399
89	Non-adiabatic molecular dynamics of molecules in the presence of strong light-matter interactions. Journal of Chemical Physics, 2019, 151, 154109.	3.0	24
90	Tuning Electronic Structure in Layered Hybrid Perovskites with Organic Spacer Substitution. Nano Letters, 2019, 19, 8732-8740.	9.1	41

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91	Halide Perovskite High-k Field Effect Transistors with Dynamically Reconfigurable Ambipolarity. , 2019, 1, 633-640.		29
92	Mod(n-m,3) Dependence of Defect-State Emission Bands in Aryl-Functionalized Carbon Nanotubes. Nano Letters, 2019, 19, 8503-8509.	9.1	22
93	Numerical tests of coherence-corrected surface hopping methods using a donor-bridge-acceptor model system. Journal of Chemical Physics, 2019, 150, 194104.	3.0	17
94	Cation Alloying Delocalizes Polarons in Lead Halide Perovskites. Journal of Physical Chemistry Letters, 2019, 10, 3516-3524.	4.6	33
95	Ground-State Geometry and Vibrations of Polyphenylenevinylene Oligomers. Journal of Physical Chemistry Letters, 2019, 10, 3232-3239.	4.6	14
96	Optical Effects of Divalent Functionalization of Carbon Nanotubes. Chemistry of Materials, 2019, 31, 6950-6961.	6.7	33
97	Intrinsic limits of defect-state photoluminescence dynamics in functionalized carbon nanotubes. Nanoscale, 2019, 11, 9125-9132.	5.6	17
98	Photoinduced non-adiabatic energy transfer pathways in dendrimer building blocks. Journal of Chemical Physics, 2019, 150, 124301.	3.0	15
99	Atomistic Simulations of Plasmon Mediated Photochemistry. ACS Symposium Series, 2019, , 239-256.	0.5	2
100	Plasmonic Hot-Carrier-Mediated Solar Energy Conversion and Tunablephotochemical Reactions. ECS Meeting Abstracts, 2019, , .	0.0	0
101	(Invited) Modeling Insights into Optical Properties of Functionalized Carbon Nanotubes. ECS Meeting Abstracts, 2019, , .	0.0	0
102	Solution-processed 2D layered perovksites for high-sensitivity X-ray detector. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, a224-a224.	0.1	0
103	Density of States Broadening in CH₃NH₃PbI₃ Hybrid Perovskites Understood from ab Initio Molecular Dynamics Simulations. ACS Energy Letters, 2018, 3, 787-793.	17.4	28
104	Composite Nature of Layered Hybrid Perovskites: Assessment on Quantum and Dielectric Confinements and Band Alignment. ACS Nano, 2018, 12, 3321-3332.	14.6	146
105	Universal Scaling of Intrinsic Resistivity in Twoâ€Dimensional Metallic Borophene. Angewandte Chemie - International Edition, 2018, 57, 4585-4589.	13.8	25
106	Correction Scheme for Comparison of Computed and Experimental Optical Transition Energies in Functionalized Single-Walled Carbon Nanotubes. Journal of Physical Chemistry Letters, 2018, 9, 2460-2468.	4.6	21
107	Light-induced lattice expansion leads to high-efficiency perovskite solar cells. Science, 2018, 360, 67-70.	12.6	554
108	Extended Lagrangian Excited State Molecular Dynamics. Journal of Chemical Theory and Computation, 2018, 14, 799-806.	5.3	8

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109	Stable Lightâ€Emitting Diodes Using Phaseâ€Pure Ruddlesdenâ€“Popper Layered Perovskites. Advanced Materials, 2018, 30, 1704217.	21.0	258
110	Lowest-Energy Crystalline Polymorphs of P3HT. Journal of Physical Chemistry C, 2018, 122, 9141-9151.	3.1	18
111	Ab initio study of two-dimensional PdPS as an ideal light harvester and promising catalyst for hydrogen evolution reaction. Materials Today Energy, 2018, 7, 136-140.	4.7	24
112	Design principles from multiscale simulations to predict nanostructure in self-assembling ionic liquids. Faraday Discussions, 2018, 206, 159-181.	3.2	9
113	Critical Role of Interface and Crystallinity on the Performance and Photostability of Perovskite Solar Cell on Nickel Oxide. Advanced Materials, 2018, 30, 1703879.	21.0	198
114	The crucial role of a spacer material on the efficiency of charge transfer processes in organic donorâ€“acceptor junction solar cells. Nanoscale, 2018, 10, 451-459.	5.6	5
115	Exciton Localization and Optical Emission in Aryl-Functionalized Carbon Nanotubes. Journal of Physical Chemistry C, 2018, 122, 1828-1838.	3.1	58
116	Single Crystal Microwires of pâ€DTS(FBTTh₂)₂ and Their Use in the Fabrication of Fieldâ€Effect Transistors and Photodetectors. Advanced Functional Materials, 2018, 28, 1702073.	14.9	22
117	Energy transfer and spatial scrambling of an exciton in a conjugated dendrimer. Physical Chemistry Chemical Physics, 2018, 20, 29648-29660.	2.8	15
118	Dipolar and charged localized excitons in carbon nanotubes. Physical Review B, 2018, 98, .	3.2	9
119	Interlayer-Decoupled Sc-Based Mxene with High Carrier Mobility and Strong Light-Harvesting Ability. Journal of Physical Chemistry Letters, 2018, 9, 6915-6920.	4.6	49
120	NEXMD Modeling of Photoisomerization Dynamics of 4-Styrylquinoline. Journal of Physical Chemistry A, 2018, 122, 9403-9411.	2.5	10
121	Geometry Distortion and Small Polaron Binding Energy Changes with Ionic Substitution in Halide Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 7130-7136.	4.6	52
122	Let Digons be Bygones: The Fate of Excitons in Curved Ï€-Systems. Journal of Physical Chemistry Letters, 2018, 9, 7123-7129.	4.6	14
123	Narrow-band single-photon emission through selective aryl functionalization of zigzag carbon nanotubes. Nature Chemistry, 2018, 10, 1089-1095.	13.6	78
124	Site-Specific Photodecomposition in Conjugated Energetic Materials. Journal of Physical Chemistry A, 2018, 122, 6055-6061.	2.5	8
125	Excited-state vibrational dynamics toward the polaron in methylammonium lead iodide perovskite. Nature Communications, 2018, 9, 2525.	12.8	129
126	Transferable Dynamic Molecular Charge Assignment Using Deep Neural Networks. Journal of Chemical Theory and Computation, 2018, 14, 4687-4698.	5.3	81

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127	Concept of Lattice Mismatch and Emergence of Surface States in Two-dimensional Hybrid Perovskite Quantum Wells. Nano Letters, 2018, 18, 5603-5609.	9.1	103
128	Discovering a Transferable Charge Assignment Model Using Machine Learning. Journal of Physical Chemistry Letters, 2018, 9, 4495-4501.	4.6	88
129	Modification of Optical Properties and Excited-State Dynamics by Linearizing Cyclic Paraphenylene Chromophores. Journal of Physical Chemistry C, 2018, 122, 16639-16648.	3.1	12
130	Solvent- and Wavelength-Dependent Photoluminescence Relaxation Dynamics of Carbon Nanotube sp³ Defect States. ACS Nano, 2018, 12, 8060-8070.	14.6	41
131	Plasmonic Hot-Carrier-Mediated Tunable Photochemical Reactions. ACS Nano, 2018, 12, 8415-8422.	14.6	75
132	Scaling law for excitons in 2D perovskite quantum wells. Nature Communications, 2018, 9, 2254.	12.8	559
133	Photoexcited Nonadiabatic Dynamics of Solvated Pushâ€“Pull Ï€-Conjugated Oligomers with the NEXMD Software. Journal of Chemical Theory and Computation, 2018, 14, 3955-3966.	5.3	39
134	Coherent exciton-vibrational dynamics and energy transfer in conjugated organics. Nature Communications, 2018, 9, 2316.	12.8	71
135	An ab initio multiple cloning approach for the simulation of photoinduced dynamics in conjugated molecules. Physical Chemistry Chemical Physics, 2018, 20, 17762-17772.	2.8	26
136	Influence of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:miÏ€</mml:mi></mml:math> -conjugated cations and halogen substitution on the optoelectronic and excitonic properties of layered hybrid perovskites. Physical Review Materials, 2018, 2, .	2.4	24
137	Solvent effects and charge transfer states in organic photovoltaics: a time-dependent density functional theory study on the PCPDTBT:PCBM low band gap system. Journal of Photonics for Energy, 2018, 8, 1.	1.3	1
138	Molecular dynamics and charge transport in organic semiconductors: a classical approach to modeling electron transfer. Chemical Science, 2017, 8, 2597-2609.	7.4	13
139	Effect of Precursor Solution Aging on the Crystallinity and Photovoltaic Performance of Perovskite Solar Cells. Advanced Energy Materials, 2017, 7, 1602159.	19.5	130
140	Extremely efficient internal exciton dissociation through edge states in layered 2D perovskites. Science, 2017, 355, 1288-1292.	12.6	830
141	Cooperative enhancement of the nonlinear optical response in conjugated energetic materials: A TD-DFT study. Journal of Chemical Physics, 2017, 146, 114308.	3.0	13
142	Photoinduced Intra- and Intermolecular Energy Transfer in ChlorophyllaDimer. Journal of Physical Chemistry B, 2017, 121, 5331-5339.	2.6	30
143	Computational Dissection of Two-Dimensional Rectangular Titanium Mononitride TiN: Auxetics and Promises for Photocatalysis. Nano Letters, 2017, 17, 4466-4472.	9.1	104
144	Electronic Delocalization, Vibrational Dynamics, and Energy Transfer in Organic Chromophores. Journal of Physical Chemistry Letters, 2017, 8, 3020-3031.	4.6	59

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145	Phonon bottleneck and long-lived excited states in Ï€-conjugated pyrene hoop. Physical Chemistry Chemical Physics, 2017, 19, 9478-9484.	2.8	12
146	Ultrafast Non-FÃ¶rster Intramolecular Donorâ€“Acceptor Excitation Energy Transfer. Journal of Physical Chemistry Letters, 2017, 8, 1688-1694.	4.6	20
147	Vibrational states of nano-confined water molecules in beryl investigated by first-principles calculations and optical experiments. Physical Chemistry Chemical Physics, 2017, 19, 30740-30748.	2.8	16
148	Low-Temperature Single Carbon Nanotube Spectroscopy of sp³ Quantum Defects. ACS Nano, 2017, 11, 10785-10796.	14.6	79
149	Multi-exciton emission from solitary dopant states of carbon nanotubes. Nanoscale, 2017, 9, 16143-16148.	5.6	5
150	First-Principles Study of Fluorescence in Silver Nanoclusters. Journal of Physical Chemistry C, 2017, 121, 23875-23885.	3.1	15
151	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.	5.5	34
152	Photoinduced dynamics in cycloparaphenylenes: planarization, electronâ€“phonon coupling, localization and intra-ring migration of the electronic excitation. Physical Chemistry Chemical Physics, 2017, 19, 30914-30924.	2.8	24
153	Charge delocalization characteristics of regioregular high mobility polymers. Chemical Science, 2017, 8, 1146-1151.	7.4	17
154	Nonadiabatic excited-state molecular dynamics: On-the-fly limiting of essential excited states. Chemical Physics, 2016, 481, 84-90.	1.9	13
155	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.	14.9	65
156	High-efficiency two-dimensional Ruddlesdenâ€“Popper perovskite solar cells. Nature, 2016, 536, 312-316.	27.8	2,767
157	Coupled wave-packets for non-adiabatic molecular dynamics: a generalization of Gaussian wave-packet dynamics to multiple potential energy surfaces. Chemical Science, 2016, 7, 4905-4911.	7.4	18
158	Photoactive Excited States in Explosive Fe(II) Tetrazine Complexes: A Time-Dependent Density Functional Theory Study. Journal of Physical Chemistry C, 2016, 120, 28762-28773.	3.1	13
159	Nonequilibrium solvent effects in Born-Oppenheimer molecular dynamics for ground and excited electronic states. Journal of Chemical Physics, 2016, 144, 154104.	3.0	7
160	Non-adiabatic excited state molecular dynamics of phenylene ethynylene dendrimer using a multiconfigurational Ehrenfest approach. Physical Chemistry Chemical Physics, 2016, 18, 10028-10040.	2.8	51
161	Polaron Stabilization by Cooperative Lattice Distortion and Cation Rotations in Hybrid Perovskite Materials. Nano Letters, 2016, 16, 3809-3816.	9.1	245
162	Through space and through bridge channels of charge transfer at p-n nano-junctions: A DFT study. Chemical Physics, 2016, 481, 144-156.	1.9	7

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163	Exciton scattering approach for optical spectra calculations in branched conjugated macromolecules. Chemical Physics, 2016, 481, 124-132.	1.9	0
164	Structurally Defined 3D Nanographene Assemblies via Bottomâ€Up Chemical Synthesis for Highly Efficient Lithium Storage. Advanced Materials, 2016, 28, 10250-10256.	21.0	72
165	Dynamics of charge at water-to-semiconductor interface: Case study of wet [0 0 1] anatase TiO2 nanowire. Chemical Physics, 2016, 481, 184-190.	1.9	5
166	Ultrafast electronic energy relaxation in a conjugated dendrimer leading to inter-branch energy redistribution. Physical Chemistry Chemical Physics, 2016, 18, 25080-25089.	2.8	29
167	Modification of optoelectronic properties of conjugated oligomers due to donor/acceptor functionalization: DFT study. Chemical Physics, 2016, 481, 133-143.	1.9	7
168	Two-Photon Absorption in Conjugated Energetic Molecules. Journal of Physical Chemistry A, 2016, 120, 4455-4464.	2.5	19
169	Interference of Interchromophoric Energy-Transfer Pathways in Ï€-Conjugated Macrocycles. Journal of Physical Chemistry Letters, 2016, 7, 4936-4944.	4.6	32
170	Advances and Promises of Layered Halide Hybrid Perovskite Semiconductors. ACS Nano, 2016, 10, 9776-9786.	14.6	351
171	Light-activated photocurrent degradation and self-healing in perovskite solar cells. Nature Communications, 2016, 7, 11574.	12.8	584
172	Carbon nanorings with inserted acenes: breaking symmetry in excited state dynamics. Scientific Reports, 2016, 6, 31253.	3.3	26
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