Dmitri Kilin

List of Publications by Year
in descending order

146	3,293	201674	189892
papers	citations	27 h-index	50 g-index

149	149	149	2800
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Breaking the Phonon Bottleneck in PbSe and CdSe Quantum Dots: Time-Domain Density Functional Theory of Charge Carrier Relaxation. ACS Nano, 2009, 3, 93-99.	14.6	236
2	Quantum Zeno Effect Rationalizes the Phonon Bottleneck in Semiconductor Quantum Dots. Physical Review Letters, 2013, 110, 180404.	7.8	230
3	Shape-controlled synthesis of silver nanoparticles: Ab initio study of preferential surface coordination with citric acid. Chemical Physics Letters, 2008, 458, 113-116.	2.6	199
4	Light-Driven and Phonon-Assisted Dynamics in Organic and Semiconductor Nanostructures. Chemical Reviews, 2015, 115, 5929-5978.	47.7	160
5	Surface Chemistry of Semiconducting Quantum Dots: Theoretical Perspectives. Accounts of Chemical Research, 2016, 49, 2127-2135.	15.6	109
6	Ab Initio Time-Domain Study of Phonon-Assisted Relaxation of Charge Carriers in a PbSe Quantum Dot. Journal of Physical Chemistry C, 2007, 111, 4871-4878.	3.1	108
7	Relaxation of Photoexcited Electrons at a Nanostructured Si(111) Surface. Journal of Physical Chemistry Letters, 2010, 1, 1073-1077.	4.6	83
8	Ab initio study of exciton transfer dynamics from a coreâ€“shell semiconductor quantum dot to a porphyrin-sensitizer. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 342-351.	3.9	67
9	Theoretical Study of Electronâ€“Phonon Relaxation in PbSe and CdSe Quantum Dots: Evidence for Phonon Memory. Journal of Physical Chemistry C, 2011, 115, 21641-21651.	3.1	60
10	Photoinduced Charge Transfer from Titania to Surface Doping Site. Journal of Physical Chemistry C, 2013, 117, 9673-9692.	3.1	59
11	Quenching of photoluminescence in a Zn-MOF sensor by nitroaromatic molecules. Journal of Materials Chemistry C, 2019, 7, 2625-2632.	5.5	54
12	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.	4.6	53
13	Excited-State Dynamics of a CsPbBr₃ Nanocrystal Terminated with Binary Ligands: Sparse Density of States with Giant Spinâ€“Orbit Coupling Suppresses Carrier Cooling. Journal of the American Chemical Society, 2019, 141, 4388-4397.	13.7	53
14	First-Principles Treatment of Photoluminescence in Semiconductors. Journal of Physical Chemistry C, 2015, 119, 27954-27964.	3.1	52
15	Photoinduced Single- and Multiple-Electron Dynamics Processes Enhanced by Quantum Confinement in Lead Halide Perovskite Quantum Dots. Journal of Physical Chemistry Letters, 2017, 8, 3032-3039.	4.6	52
16	Surface Photovoltage at Nanostructures on Si Surfaces: Ab Initio Results. Journal of Physical Chemistry C, 2009, 113, 3530-3542.	3.1	51
17	Optical Properties of Doped Silicon Quantum Dots with Crystalline and Amorphous Structures. Journal of Physical Chemistry C, 2011, 115, 19529-19537.	3.1	45
18	Universal Size-Dependent Stokes Shifts in Lead Halide Perovskite Nanocrystals. Journal of Physical Chemistry Letters, 2020, 11, 4937-4944.	4.6	44

#	Article	IF	Citations
19	Bright Silicon Nanocrystals from a Liquid Precursor: Quasi-Direct Recombination with High Quantum Yield. ACS Nano, 2020, 14, 3858-3867.	14.6	43
20	Photoinduced Conductivity of a Porphyrinâ"Gold Composite Nanowire. Journal of Physical Chemistry A, 2009, 113, 4549-4556.	2.5	37
21	Abrupt Size Partitioning of Multimodal Photoluminescence Relaxation in Monodisperse Silicon Nanocrystals. ACS Nano, 2017, 11, 1597-1603.	14.6	34
22	Wave packet interferometry for short-time electronic energy transfer: Multidimensional optical spectroscopy in the time domain. Journal of Chemical Physics, 2003, 118, 46-61.	3.0	32
23	Computational simulation of the pâ€n doped silicon quantum dot. International Journal of Quantum Chemistry, 2012, 112, 3879-3888.	2.0	32
24	Electron-nuclear correlations for photo-induced dynamics in molecular dimers. Journal of Chemical Physics, 2004, 120, 11209-11223.	3.0	31
25	Modeling the Photovoltage of Doped Si Surfaces. Journal of Physical Chemistry C, 2011, 115, 770-775.	3.1	31
26	DFT Calculation of Russellâ€"Saunders Splitting for Lanthanide Ions Doped in Hexagonal (Î²)-NaYF4 Nanocrystals. Journal of Physical Chemistry C, 2013, 117, 17177-17185.	3.1	31
27	Sequential hydrogen dissociation from a charged Pt₁₃H₂₄ cluster modeled by ab initio molecular dynamics. International Journal of Quantum Chemistry, 2012, 112, 3896-3903.	2.0	29
28	Photoabsorbance and Photovoltage of Crystalline and Amorphous Silicon Slabs with Silver Adsorbates. Journal of Physical Chemistry C, 2012, 116, 25525-25536.	3.1	28
29	Excited State Dynamics of Ru₁₀ Cluster Interfacing Anatase TiO₂(101) Surface and Liquid Water. Journal of Physical Chemistry Letters, 2014, 5, 2823-2829.	4.6	28
30	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
31	Thermal equation of state of solid naphthalene to 13 GPa and 773 K: In situ X-ray diffraction study and first principles calculations. Journal of Chemical Physics, 2014, 140, 164508.	3.0	26
32	Time-dependent excited-state molecular dynamics of photodissociation of lanthanide complexes for laser-assisted metal-organic chemical vapour deposition. Molecular Physics, 2014, 112, 508-517.	1.7	26
33	Charge Transfer, Luminescence, and Phonon Bottleneck in TiO₂ Nanowires Computed by Eigenvectors of Liouville Superoperator. Journal of Chemical Theory and Computation, 2014, 10, 3996-4005.	5.3	26
34	Photofragmentation of the Gas-Phase Lanthanum Isopropylcyclopentadienyl Complex: Computational Modeling vs Experiment. Journal of Physical Chemistry A, 2015, 119, 10838-10848.	2.5	26
35	Photoinduced Charge Transfer versus Fragmentation Pathways in Lanthanum Cyclopentadienyl Complexes. Journal of Chemical Theory and Computation, 2017, 13, 4281-4296.	5.3	26
36	Ab initiostudy of the photocurrent at the Au/Si metalâ€"semiconductor nanointerface. Molecular Physics, 2015, 113, 327-335.	1.7	25

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37	One-pot synthesis of enzyme@metalâ€“organic material (MOM) biocomposites for enzyme biocatalysis. Green Chemistry, 2021, 23, 4466-4476.	9.0	25
38	Computational modeling of wet TiO₂ (001) anatase surfaces functionalized by transition metal doping. International Journal of Quantum Chemistry, 2012, 112, 3867-3873.	2.0	24
39	First-Principles Study of Optoelectronic Properties of the Noble Metal (Ag and Pd) Doped BiOX (X = F,) Tj ETQq1 1 0.784314 rgBT /Over	3.5	24
40	Atomic modeling of surface photovoltage: Application to Si(1 1 1):H. Chemical Physics Letters, 2008, 461, 266-270.	2.6	23
41	Dynamics of charge transfer at Au/Si metal-semiconductor nano-interface. Molecular Physics, 2014, 112, 474-484.	1.7	23
42	Multiple exciton generation in silicon quantum dot arrays: density functional perturbation theory computation. Molecular Physics, 2014, 112, 430-440.	1.7	21
43	Enhancing Silicon Nanocrystal Photoluminescence through Temperature and Microstructure. Journal of Physical Chemistry C, 2016, 120, 18909-18916.	3.1	21
44	Photofragmentation of Tetranitromethane: Spin-Unrestricted Time-Dependent Excited-State Molecular Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 3185-3192.	4.6	21
45	Structure-Driven Photoluminescence Enhancement in a Zn-Based Metalâ€“Organic Framework. Chemistry of Materials, 2019, 31, 7933-7940.	6.7	21
46	Electron Transfer in Porphyrin Complexes in Different Solvents. Journal of Physical Chemistry A, 2000, 104, 5413-5421.	2.5	20
47	Direct and indirect electron transfer at a semiconductor surface with an adsorbate: Theory and application to Ag3Si(111):H. Journal of Chemical Physics, 2010, 132, 114702.	3.0	20
48	Anatase (100) thin film surface computational model for photoelectrochemical cell. International Journal of Quantum Chemistry, 2012, 112, 3874-3878.	2.0	20
49	Electron dynamics in charged wet TiO2anatase (001) surface functionalised by ruthenium ions. Molecular Physics, 2014, 112, 441-452.	1.7	20
50	Role of Lead Vacancies for Optoelectronic Properties of Lead-Halide Perovskites. Journal of Physical Chemistry C, 2018, 122, 5216-5226.	3.1	20
51	Understanding of Light Absorption Properties of the N-Doped Graphene Oxide Quantum Dot with TD-DFT. Journal of Physical Chemistry C, 2021, 125, 14979-14990.	3.1	20
52	Optical properties of the Si(111):H surface with adsorbed Ag clusters. International Journal of Quantum Chemistry, 2009, 109, 3694-3704.	2.0	19
53	Non-collinear spin DFT for lanthanide ions in doped hexagonal NaYF₄. Molecular Physics, 2014, 112, 546-556.	1.7	19
54	Spin Unrestricted Excited State Relaxation Study of Vanadium(IV)-Doped Anatase. Journal of Physical Chemistry C, 2016, 120, 5890-5905.	3.1	19

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55	Optical properties of amorphous and crystalline silicon surfaces functionalized with Ag_n adsorbates. International Journal of Quantum Chemistry, 2010, 110, 3005-3014.	2.0	18
56	Unexpected high binding energy of CO₂ on CH₃NH₃PbI₃ lead-halide organicâ€“inorganic perovskites via bicarbonate formation. Chemical Communications, 2018, 54, 9949-9952.	4.1	18
57	Density matrix treatment of combined instantaneous and delayed dissipation for an electronically excited adsorbate on a solid surface. Journal of Chemical Physics, 2009, 131, 144106.	3.0	17
58	Electronic structure and hot carrier relaxation in âŸ¨001âŸ© anatase TiO₂nanowire. Molecular Physics, 2014, 112, 539-545.	1.7	17
59	Comparison of two models for bridge-assisted charge transfer. Journal of Luminescence, 1999, 83-84, 235-240.	3.1	15
60	Electronic properties of nickel-doped TiO2 anatase. Journal of Physics Condensed Matter, 2015, 27, 134207.	1.8	15
61	First-Principles Study of Fluorescence in Silver Nanoclusters. Journal of Physical Chemistry C, 2017, 121, 23875-23885.	3.1	15
62	Spinor Dynamics in Pristine and Mn2+-Doped CsPbBr3 NC: Role of Spinâ€“Orbit Coupling in Ground- and Excited-State Dynamics. Journal of Physical Chemistry C, 2018, 122, 26196-26213.	3.1	15
63	Theoretical predictions on efficiency of bi-exciton formation and dissociation in chiral carbon nanotubes. Journal of Chemical Physics, 2016, 145, 154112.	3.0	14
64	Photofragmentation Pathways for Gas-Phase Lanthanide Tris(isopropylcyclopentadienyl) Complexes. Organometallics, 2016, 35, 3461-3473.	2.3	14
65	Hole Transfer in Dye-Sensitized Cesium Lead Halide Perovskite Photovoltaics: Effect of Interfacial Bonding. Journal of Physical Chemistry C, 2017, 121, 20113-20125.	3.1	14
66	Unraveling Photodimerization of Cyclohexasilane from Molecular Dynamics Studies. Journal of Physical Chemistry Letters, 2018, 9, 4349-4354.	4.6	14
67	Defect Tolerance Mechanism Revealed! Influence of Polaron Occupied Surface Trap States on CsPbBr₃ Nanocrystal Photoluminescence: Ab Initio Excited-State Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 7224-7236.	5.3	14
68	First-Principles Studies of Photoinduced Charge Transfer in Noncovalently Functionalized Carbon Nanotubes. Journal of Physical Chemistry C, 2013, 117, 17909-17918.	3.1	13
69	Proton reduction at surface of transition metal nanocatalysts. Molecular Simulation, 2015, 41, 134-145.	2.0	13
70	Photoinduced Charge Transfer at Interfaces of Carbon Nanotube and Lead Selenide Nanowire. Journal of Physical Chemistry C, 2016, 120, 23197-23206.	3.1	13
71	Brightly Luminescent CsPbBr₃ Nanocrystals through Ultracentrifugation. Journal of Physical Chemistry Letters, 2020, 11, 7133-7140.	4.6	13
72	Photoinduced Vibrational Coherence Transfer in Molecular Dimers. Journal of Physical Chemistry A, 2007, 111, 10212-10219.	2.5	12

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73	Amorphous silicon nanomaterials: Quantum dots versus nanowires. Journal of Renewable and Sustainable Energy, 2013, 5, .	2.0	12
74	Multiple exciton generation in chiral carbon nanotubes: Density functional theory based computation. Journal of Chemical Physics, 2017, 147, 154106.	3.0	12
75	Induced Chirality in Halide Perovskite Clusters through Surface Chemistry. Journal of Physical Chemistry Letters, 2022, 13, 686-693.	4.6	12
76	Electronic Properties of Silver Doped TiO2 Anatase (100) Surface. ACS Symposium Series, 2013, , 187-218.	0.5	11
77	Singlet fission in chiral carbon nanotubes: Density functional theory based computation. Journal of Chemical Physics, 2017, 147, 034106.	3.0	11
78	Spectral Signatures of Positive and Negative Polarons in Lead-Halide Perovskite Nanocrystals. Journal of Physical Chemistry C, 2020, 124, 1027-1041.	3.1	11
79	Nonradiative Relaxation Dynamics of a Cesium Lead Halide Perovskite Photovoltaic Architecture: Effect of External Electric Fields. Journal of Physical Chemistry Letters, 2020, 11, 9983-9989.	4.6	11
80	ATOMISTIC SIMULATION OF DISSIPATIVE CHARGE CARRIER DYNAMICS FOR PHOTOCATALYSIS. Materials Research Society Symposia Proceedings, 2012, 1390, 172.	0.1	10
81	Optical properties of host material for phosphor computational modeling. International Journal of Quantum Chemistry, 2012, 112, 3889-3895.	2.0	10
82	Molecular dynamics in finding nonadiabatic coupling for Î²-NaYF₄: Ce³⁺nanocrystals. Molecular Physics, 2015, 113, 385-391.	1.7	10
83	Charge Transfer Mechanism in Titanium-Doped Microporous Silica for Photocatalytic Water-Splitting Applications. Catalysts, 2016, 6, 34.	3.5	10
84	Molecular dynamics of laser-assisted decomposition of unstable molecules at the surface of carbon nanotubes: case study of CH2(NO2)2 on CNT(4,0). Molecular Physics, 2017, 115, 674-682.	1.7	10
85	Coupling between Emissive Defects on Carbon Nanotubes: Modeling Insights. Journal of Physical Chemistry Letters, 2021, 12, 7846-7853.	4.6	10
86	Competition between electron transfer and energy migration in self-assembled porphyrin triads. Materials Science and Engineering C, 2001, 18, 99-111.	7.3	9
87	Computational studies of the optical properties of silicon compounds bonding to silver atoms and with group III and V substituents. International Journal of Quantum Chemistry, 2010, 110, 3086-3094.	2.0	9
88	Electronic structure and optical absorbance of doped amorphous silicon slabs. International Journal of Quantum Chemistry, 2012, 112, 300-313.	2.0	9
89	Modeling the surface photovoltage of silicon slabs with varying thickness. Journal of Physics Condensed Matter, 2015, 27, 134204.	1.8	9
90	Dynamics of Charge Transfer and Multiple Exciton Generation in the Doped Silicon Quantum Dotâ€“Carbon Nanotube System: Density Functional Theory-Based Computation. Journal of Physical Chemistry Letters, 2018, 9, 5759-5764.	4.6	9

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91	Photoexcited Electron Lifetimes Influenced by Momentum Dispersion in Silicon Nanowires. Journal of Physical Chemistry C, 2019, 123, 7457-7466.	3.1	9
92	Photofragmentation of Gas-Phase Lanthanide Cyclopentadienyl Complexes: Experimental and Time-Dependent Excited-State Molecular Dynamics. Organometallics, 2014, 33, 1574-1586.	2.3	8
93	Spin Unrestricted Nonradiative Relaxation Dynamics of Cobalt-Doped Anatase Nanowire. Journal of Physical Chemistry C, 2017, 121, 16110-16125.	3.1	8
94	Photoinduced dynamics to photoluminescence in Ln³⁺ (Ln = Ce, Pr) doped Î²-NaYF₄ nanocrystals computed in basis of non-collinear spin DFT with spin-orbit coupling. Molecular Physics, 2018, 116, 697-707.	1.7	8
95	Role of Cation-Anion Organic Ligands for Optical Properties of Fully Inorganic Perovskite Quantum Dots. MRS Advances, 2018, 3, 3255-3261.	0.9	8
96	First-Principles Molecular Dynamics of Monomethylhydrazine and Nitrogen Dioxide. Journal of Physical Chemistry Letters, 2019, 10, 2394-2399.	4.6	8
97	Electron dynamics of solvated titanium hydroxide. Molecular Physics, 2015, 113, 397-407.	1.7	7
98	Enhanced multiple exciton generation in amorphous silicon nanowires and films. Molecular Physics, 0, , 1-15.	1.7	7
99	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
100	Mathematical modeling of gas desorption from a metalâ€“organic supercontainer cavity filled with stored N2gas at critical limits. RSC Advances, 2017, 7, 11180-11190.	3.6	7
101	First-principles study of electron dynamics with explicit treatment of momentum dispersion on Si nanowires along different directions. Molecular Physics, 2019, 117, 2293-2302.	1.7	7
102	First-Principles Study on the Electronic Properties of PDPP-Based Conjugated Polymer via Density Functional Theory. Journal of Physical Chemistry B, 2021, 125, 8953-8964.	2.6	7
103	Adsorption patterns of caffeic acid on titania: affinity, charge transfer and sunscreen applications. Molecular Physics, 0, , 1-11.	1.7	6
104	First-Principles Study of Charge Carrier Dynamics with Explicit Treatment of Momentum Dispersion on Si Nanowires along <211> crystallographic Directions. MRS Advances, 2018, 3, 3477-3482.	0.9	6
105	Silver Nanoparticles for Catalysis of Hydrogen Peroxide Decomposition: Atomistic Modeling. Materials Research Society Symposia Proceedings, 2015, 1787, 21-25.	0.1	5
106	Time-resolved electronic and optical properties of a thiolate-protected Au₃₈nanocluster. Molecular Physics, 2015, 113, 408-417.	1.7	5
107	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
108	Quantitative Attachment of Bimetal Combinations of Transition-Metal Ions to the Surface of TiO₂ Nanorods. Langmuir, 2018, 34, 5422-5434.	3.5	5

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109	Adsorption of Formic Acid on CH3NH3PbI3 Leadâ€“Halide Organicâ€“Inorganic Perovskites. Journal of Physical Chemistry C, 2019, 123, 22873-22886.	3.1	5
110	Decoherence for phase-sensitive relaxation. Journal of Luminescence, 2000, 92, 13-25.	3.1	4
111	Photoinduced Electron Transfer Dynamics for Self-Assembled Porphyrin Arrays in Solutions and Films. Molecular Crystals and Liquid Crystals, 2001, 361, 83-88.	0.3	4
112	Electron Dynamics of Solvated Ti(OH)4. Materials Research Society Symposia Proceedings, 2014, 1647, 1.	0.1	4
113	Ab Initio Analysis of Charge Carrier Dynamics in Organic-Inorganic Lead Halide Perovskite Solar Cells. Materials Research Society Symposia Proceedings, 2015, 1776, 19-29.	0.1	4
114	Relationship between Site Symmetry, Spin State, and Doping Concentration for Co(II) or Co(III) in Î²-NaYF₄. Journal of Physical Chemistry C, 2016, 120, 7785-7794.	3.1	4
115	Molecular dynamics of reactions between (4,0) zigzag carbon nanotube and hydrogen peroxide under extreme conditions. Molecular Physics, 2018, 116, 708-716.	1.7	4
116	Role of Pb2+ Adsorbents on the Opto-Electronic Properties of a CsPbBr3 Nanocrystal: A DFT Study. MRS Advances, 2019, 4, 1981-1988.	0.9	4
117	Synthesis of Holey Graphene Nanoparticle Compounds. ACS Applied Materials & Interfaces, 2020, 12, 36513-36522.	8.0	4
118	Mechanisms of Photoluminescence in Copper-Containing Fluoride Borate Crystals. Journal of Physical Chemistry C, 0, , .	3.1	4
119	Influence of phase-sensitive interaction on the decoherence process in molecular systems. Journal of Luminescence, 1998, 76-77, 433-436.	3.1	3
120	Anatase TiO2 Nanowires, Thin Films, and Surfaces: Ab initio Studies of Electronic Properties and Non-adiabatic Excited State Dynamics. Materials Research Society Symposia Proceedings, 2014, 1659, 129-134.	0.1	3
121	Elucidating the role of non-radiative processes in charge transfer of coreâ€“shell Siâ€“SiO₂Ânanoparticles. Molecular Physics, 2014, 112, 422-429.	1.7	3
122	Cobalt-doped TiO2: a computational analysis of dopant placement and charge transfer direction on thin film anatase. Molecular Physics, 2015, , 1-15.	1.7	3
123	Single Site Metal Ions on the Surface of TiO2 Nanorods - A Platform for Theoretical and Experimental Investigation. ACS Symposium Series, 2015, , 103-116.	0.5	3
124	Hot Carrier Dynamics at Ligated Silicon(111) Surfaces: A Computational Study. Journal of Physical Chemistry Letters, 2021, 12, 7504-7511.	4.6	3
125	Size-Dependent Doping Synergy and Dual-Color Emission in CsPb1-xMnxCl3 Nanocrystals. Journal of Physical Chemistry C, 2021, 125, 18849-18856.	3.1	3
126	Electronic Relaxation of Photoexcited Open and Closed Shell Adsorbates on Semiconductors: Ag and Ag2 on TiO2. Journal of Chemical Physics, 2022, 156, 104705.	3.0	3

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127	Photoluminescence of Cis-Polyacetylene Semiconductor Material. Applied Sciences (Switzerland), 2022, 12, 2830.	2.5	3
128	Electronic confinement effects and optical properties of multilayer slabs of silicon: numerical model studies. , 2009, , .		2
129	Anions vs. Cations of Pt13H24 Cluster Models: Ab Initio Molecular Dynamics Investigation of Electronic Properties and Photocatalytic Activity. ACS Symposium Series, 2013, , 173-185.	0.5	2
130	Electronic and spectral properties of ametal-organic super container molecule by single point DFT. Molecular Physics, 2015, , 1-6.	1.7	2
131	A Computational Study of the Combustion of Hydrazine with Dinitrogen Tetroxide. Journal of Nanotoxicology and Nanomedicine, 2017, 2, 12-30.	0.7	2
132	Time-resolved Optical Properties of SiNW Oriented in <211> Crystallographic Direction. MRS Advances, 2019, 4, 2009-2014.	0.9	2
133	Molecular Dynamics Study of the Photodegradation of Polymeric Chains. Journal of Physical Chemistry Letters, 2022, 13, 4374-4380.	4.6	2
134	First-Principles Study on Optoelectronic Properties of Fe-Doped Montmorillonite Clay. Journal of Physical Chemistry Letters, 2022, 13, 4257-4262.	4.6	2
135	Calculating electronic properties of the Si:SiO<inf>2</inf> interface using density functional theory with periodical boundary condition. , 2013, , .		1
136	Spin-Unrestricted and Spinor Nonradiative Relaxation Dynamics in Functionalized Semiconductors. ACS Symposium Series, 2019, , 1-22.	0.5	1
137	Magnetic-Field-Driven Electron Dynamics in Graphene. Journal of Physical Chemistry Letters, 2021, 12, 4749-4754.	4.6	1
138	Effect of ligand groups on photoexcited charge carrier dynamics at the perovskite/TiO₂ interface. RSC Advances, 2021, 12, 78-87.	3.6	1
139	Photo-Induced Charge Transfer of Fullerene and Non-Fullerene Conjugated Polymer Blends via Ab Initio Excited-State Dynamics. Journal of Physical Chemistry C, 2022, 126, 12015-12024.	3.1	1
140	Spatially non-uniform field response in arrays of silicon quantum dots: DFT computation. , 2013, , .		0
141	Toward First-Principles Description of Carrier Relaxation in Nanoparticles. ACS Symposium Series, 2015, , 201-213.	0.5	0
142	A Technology-Centered, Project-Based Approach in Physical and Computational Chemistry Curriculum. ACS Symposium Series, 2019, , 143-163.	0.5	0
143	Comprehensive Study of Multiple Exciton Generation in Chiral Carbon Nanotubes Using Many-Body Perturbation Theory Based on Density Functional Theory Simulations. ACS Symposium Series, 2019, , 157-179.	0.5	0
144	Excited state dynamics in a sodium and iodine co-doped lead telluride nanowire. Molecular Physics, 2021, 119, e1874557.	1.7	0

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145	Electronic structure of semiconductor nanoparticles from stochastic evaluation of imaginary-time path integral. Physical Review Research, 2021, 3, .	3.6	0
146	Quantitative Experimental and Theoretical Analysis of Photoinduced Relaxation Processes in Self-Assembled Porphyrin Triads. Macroheterocycles, 2020, 13, 130-141.	0.5	0