David A Egger

List of Publications by Year
in descending order

196 papers	19,866 citations	18887 64 h-index	12638 137 g-index
198 all docs	198 docs citations	198 times ranked	21696 citing authors

#	Article	IF	Citations
1	Exciton Binding Energy and Nonhydrogenic Rydberg Series in Monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>WS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></ Physical Review Letters, 2014, 113, 076802.	2.9	1,814
2	Colloquium : Excitons in atomically thin transition metal dichalcogenides. Reviews of Modern Physics, 2018, 90, .	16.4	1,292
3	Hybrid organicâ€"inorganic perovskites: low-cost semiconductors with intriguing charge-transport properties. Nature Reviews Materials, 2016, 1, .	23.3	1,173
4	Measurement of the optical dielectric function of monolayer transition-metal dichalcogenides:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mm xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:mi mathvariant="normal">S</mml:mi><mml:msub><mml:mi mathvariant="normal">e</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>,<mml:math	1.1	1,017
5	Theory of neutral and charged excitons in monolayer transition metal dichalcogenides. Physical Review B, 2013, 88, .	1.1	737
6	Observation of biexcitons in monolayer WSe2. Nature Physics, 2015, 11, 477-481.	6.5	531
7	Coulomb engineering of the bandgap and excitons in two-dimensional materials. Nature Communications, 2017, 8, 15251.	5.8	526
8	Local Polar Fluctuations in Lead Halide Perovskite Crystals. Physical Review Letters, 2017, 118, 136001.	2.9	489
9	Valley Splitting and Polarization by the Zeeman Effect in Monolayer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>MoSe</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></ Physical Review Letters, 2014, 113, 266804.	2.9	395
10	Hybrid Organicâ€"Inorganic Perovskites (HOIPs): Opportunities and Challenges. Advanced Materials, 2015, 27, 5102-5112.	11.1	372
11	Irreversible reorganization in a supercooled liquid originates from localized soft modes. Nature Physics, 2008, 4, 711-715.	6.5	367
12	Population inversion and giant bandgap renormalization in atomically thin WS2 layers. Nature Photonics, 2015, 9, 466-470.	15.6	366
13	Excitonic linewidth and coherence lifetime in monolayer transition metal dichalcogenides. Nature Communications, 2016, 7, 13279.	5.8	360
14	Valence and Conduction Band Densities of States of Metal Halide Perovskites: A Combined Experimentalâ€"Theoretical Study. Journal of Physical Chemistry Letters, 2016, 7, 2722-2729.	2.1	333
15	Electrical Tuning of Exciton Binding Energies in Monolayer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>WS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></ Physical Review Letters, 2015, 115, 126802.	2.9	323
16	Optical phonons in methylammonium lead halide perovskites and implications for charge transport. Materials Horizons, 2016, 3, 613-620.	6.4	299
17	Probing Interlayer Interactions in Transition Metal Dichalcogenide Heterostructures by Optical Spectroscopy: MoS₂/WS₂ and MoSe₂/WSe₂. Nano Letters, 2015, 15, 5033-5038.	4.5	277
18	Excitons in ultrathin organic-inorganic perovskite crystals. Physical Review B, 2015, 92, .	1.1	263

#	Article	IF	Citations
19	The Quantum Coherent Mechanism for Singlet Fission: Experiment and Theory. Accounts of Chemical Research, 2013, 46, 1321-1329.	7.6	262
20	High Chloride Doping Levels Stabilize the Perovskite Phase of Cesium Lead Iodide. Nano Letters, 2016, 16, 3563-3570.	4.5	247
21	Absence of Diffusion in an Interacting System of Spinless Fermions on a One-Dimensional Disordered Lattice. Physical Review Letters, 2015, 114, 100601.	2.9	246
22	What Remains Unexplained about the Properties of Halide Perovskites?. Advanced Materials, 2018, 30, e1800691.	11.1	231
23	Momentum-space indirect interlayer excitons in transition-metal dichalcogenide van der Waals heterostructures. Nature Physics, 2018, 14, 801-805.	6.5	229
24	Hybrid Organicâ€“Inorganic Perovskites on the Move. Accounts of Chemical Research, 2016, 49, 573-581.	7.6	227
25	Dielectric disorder in two-dimensional materials. Nature Nanotechnology, 2019, 14, 832-837.	15.6	223
26	Role of Dispersive Interactions in Determining Structural Properties of Organicâ€“Inorganic Halide Perovskites: Insights from First-Principles Calculations. Journal of Physical Chemistry Letters, 2014, 5, 2728-2733.	2.1	199
27	Are Mobilities in Hybrid Organicâ€“Inorganic Halide Perovskites Actually â€œHighâ€?. Journal of Physical Chemistry Letters, 2015, 6, 4754-4757.	2.1	197
28	Exciton Diffusion and Halo Effects in Monolayer Semiconductors. Physical Review Letters, 2018, 120, 207401.	2.9	193
29	Direct Observation of Ultrafast Exciton Formation in a Monolayer of WSe₂. Nano Letters, 2017, 17, 1455-1460.	4.5	171
30	Microscopic theory of singlet exciton fission. III. Crystalline pentacene. Journal of Chemical Physics, 2014, 141, 074705.	1.2	160
31	Light-induced picosecond rotational disordering of the inorganic sublattice in hybrid perovskites. Science Advances, 2017, 3, e1602388.	4.7	149
32	The Role of Electronic and Phononic Excitation in the Optical Response of Monolayer WS₂ after Ultrafast Excitation. Nano Letters, 2017, 17, 644-651.	4.5	143
33	Transient superconductivity from electronic squeezing of optically pumped phonons. Nature Physics, 2017, 13, 479-483.	6.5	139
34	Taming the Dynamical Sign Problem in Real-Time Evolution of Quantum Many-Body Problems. Physical Review Letters, 2015, 115, 266802.	2.9	138
35	Theory of Hydrogen Migration in Organicâ€“Inorganic Halide Perovskites. Angewandte Chemie - International Edition, 2015, 54, 12437-12441.	7.2	134
36	Outer-valence Electron Spectra of Prototypical Aromatic Heterocycles from an Optimally Tuned Range-Separated Hybrid Functional. Journal of Chemical Theory and Computation, 2014, 10, 1934-1952.	2.3	128

#	Article	IF	Citations
37	Reliable Energy Level Alignment at Physisorbed Moleculeâ€“Metal Interfaces from Density Functional Theory. Nano Letters, 2015, 15, 2448-2455.	4.5	112
38	Numerically exact long-time magnetization dynamics at the nonequilibrium Kondo crossover of the Anderson impurity model. Physical Review B, 2013, 87, .	1.1	111
39	Dynamic emission Stokes shift and liquid-like dielectric solvation of band edge carriers in lead-halide perovskites. Nature Communications, 2019, 10, 1175.	5.8	111
40	Accurate Force Field Development for Modeling Conjugated Polymers. Journal of Chemical Theory and Computation, 2012, 8, 4556-4569.	2.3	109
41	Triplet Separation Drives Singlet Fission after Femtosecond Correlated Triplet Pair Production in Rubrene. Journal of the American Chemical Society, 2017, 139, 11745-11751.	6.6	107
42	Roadmap on organicâ€“inorganic hybrid perovskite semiconductors and devices. APL Materials, 2021, 9, .	2.2	102
43	How Lattice and Charge Fluctuations Control Carrier Dynamics in Halide Perovskites. Nano Letters, 2018, 18, 8041-8046.	4.5	97
44	Perylene Diimide-Based Hj- and hJ-Aggregates: The Prospect of Exciton Band Shape Engineering in Organic Materials. Journal of Physical Chemistry C, 2019, 123, 20567-20578.	1.5	91
45	The Effects of Embedded Dipoles in Aromatic Selfâ€Assembled Monolayers. Advanced Functional Materials, 2015, 25, 3943-3957.	7.8	90
46	Binding energies and spatial structures of small carrier complexes in monolayer transition-metal dichalcogenides via diffusion Monte Carlo. Physical Review B, 2015, 92, .	1.1	88
47	Impact of Small Phonon Energies on the Charge-Carrier Lifetimes in Metal-Halide Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 939-946.	2.1	88
48	Quantum fluctuations can promote or inhibit glassÂformation. Nature Physics, 2011, 7, 134-137.	6.5	84
49	Effect of Solid-State Polarization on Charge-Transfer Excitations and Transport Levels at Organic Interfaces from a Screened Range-Separated Hybrid Functional. Journal of Physical Chemistry Letters, 2017, 8, 3277-3283.	2.1	84
50	Unbiasing fermionic quantum Monte Carlo with a quantum computer. Nature, 2022, 603, 416-420.	13.7	84
51	Correlation of Local Order with Particle Mobility in Supercooled Liquids Is Highly System Dependent. Physical Review Letters, 2014, 113, 157801.	2.9	83
52	Greenâ€™s Functions from Real-Time Bold-Line MonteÂCarlo Calculations: Spectral Properties of the Nonequilibrium Anderson Impurity Model. Physical Review Letters, 2014, 112, 146802.	2.9	80
53	Constructing the Electronic Structure of CH₃NH₃PbI₃ and CH₃NH₃PbBr₃ Perovskite Thin Films from Single-Crystal Band Structure Measurements. Journal of Physical Chemistry Letters, 2019, 10, 601-609.	2.1	78
54	Vibronic exciton theory of singlet fission. I. Linear absorption and the anatomy of the correlated triplet pair state. Journal of Chemical Physics, 2017, 146, 174703.	1.2	77

#	Article	IF	Citations
55	Dynamic shortening of disorder potentials in anharmonic halide perovskites. Nature Communications, 2019, 10, 3141.	5.8	74
56	Exciton diffusion in monolayer semiconductors with suppressed disorder. Physical Review B, 2020, 101, .	1.1	74
57	The Significance of Polarons and Dynamic Disorder in Halide Perovskites. ACS Energy Letters, 2021, 6, 2162-2173.	8.8	74
58	Perovskite Solar Cells: Do We Know What We Do Not Know?. Journal of Physical Chemistry Letters, 2015, 6, 279-282.	2.1	71
59	Work-Function Modification beyond Pinning: When Do Molecular Dipoles Count?. Nano Letters, 2010, 10, 4369-4374.	4.5	70
60	Zeeman Splitting and Inverted Polarization of Biexciton Emission in Monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>WS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:m Physical Review Letters, 2018, 121, 057402.	2.9	70
61	Understanding the Adsorption of CuPc and ZnPc on Noble Metal Surfaces by Combining Quantum-Mechanical Modelling and Photoelectron Spectroscopy. Molecules, 2014, 19, 2969-2992.	1.7	69
62	Bright and dark singlet excitons via linear and two-photon spectroscopy in monolayer transition-metal dichalcogenides. Physical Review B, 2015, 92, .	1.1	68
63	Optical and Excitonic Properties of Atomically Thin Transition-Metal Dichalcogenides. Annual Review of Condensed Matter Physics, 2018, 9, 379-396.	5.2	68
64	Vibronic exciton theory of singlet fission. III. How vibronic coupling and thermodynamics promote rapid triplet generation in pentacene crystals. Journal of Chemical Physics, 2018, 148, 244701.	1.2	67
65	Bold-line diagrammatic Monte Carlo method: General formulation and application to expansion around the noncrossing approximation. Physical Review B, 2010, 82, .	1.1	64
66	Exciton Propagation and Halo Formation in Two-Dimensional Materials. Nano Letters, 2019, 19, 7317-7323.	4.5	64
67	Microscopic Dynamics of Supercooled Liquids from First Principles. Physical Review Letters, 2015, 115, 205701.	2.9	62
68	On Achieving High Accuracy in Quantum Chemical Calculations of 3d Transition Metal-Containing Systems: A Comparison of Auxiliary-Field Quantum Monte Carlo with Coupled Cluster, Density Functional Theory, and Experiment for Diatomic Molecules. Journal of Chemical Theory and Computation, 2019, 15, 2346-2358.	2.3	62
69	Comparing time-dependent density functional theory with many-body perturbation theory for semiconductors: Screened range-separated hybrids and the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml plus Bethe-Salpeter approach. Physical Review Materials, 2019, 3, .	0.9	61
70	Length- and Thickness-Dependent Optical Response of Liquid-Exfoliated Transition Metal Dichalcogenides. Chemistry of Materials, 2019, 31, 10049-10062.	3.2	57
71	Single-crystal-to-single-crystal intercalation of a low-bandgap superatomic crystal. Nature Chemistry, 2017, 9, 1170-1174.	6.6	56
72	Intrinsic lifetime of higher excitonic states in tungsten diselenide monolayers. Nanoscale, 2019, 11, 12381-12387.	2.8	56

#	Article	IF	Citations
73	Numerically exact long-time behavior of nonequilibrium quantum impurity models. Physical Review B, 2011, 84, .	1.1	55
74	Broad Tunability of Carrier Effective Masses in Two-Dimensional Halide Perovskites. ACS Energy Letters, 2020, 5, 3609-3616.	8.8	54
75	Vibronic exciton theory of singlet fission. II. Two-dimensional spectroscopic detection of the correlated triplet pair state. Journal of Chemical Physics, 2017, 146, 174704.	1.2	53
76	Breakdown of the Static Picture of Defect Energetics in Halide Perovskites: The Case of the Br Vacancy in CsPbBr₃. Journal of Physical Chemistry Letters, 2019, 10, 4490-4498.	2.1	52
77	Green's functions from real-time bold-line Monte Carlo. Physical Review B, 2014, 89, .	1.1	51
78	Enhancement of Excitonâ€“Phonon Scattering from Monolayer to Bilayer WS₂. Nano Letters, 2018, 18, 6135-6143.	4.5	50
79	Comparison of Dynamical Heterogeneity in Hard-Sphere and Attractive Glass Formersâ€. Journal of Physical Chemistry B, 2005, 109, 14654-14658.	1.2	49
80	Approximate but accurate quantum dynamics from the Mori formalism: I. Nonequilibrium dynamics. Journal of Chemical Physics, 2016, 144, 184104.	1.2	48
81	Inchworm Monte Carlo for exact non-adiabatic dynamics. I. Theory and algorithms. Journal of Chemical Physics, 2017, 146, 054105.	1.2	47
82	Depletion of Two-Level Systems in Ultrastable Computer-Generated Glasses. Physical Review Letters, 2020, 124, 225901.	2.9	47
83	Transition voltages respond to synthetic reorientation of embedded dipoles in self-assembled monolayers. Chemical Science, 2016, 7, 781-787.	3.7	46
84	Exciton broadening in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>WS</mml:mi><mml:mn>2</mml:mn></mml:msub></mm /graphene heterostructures. Physical Review B, 2017, 96, .	1.1	46
85	Removing instabilities in the hierarchical equations of motion: Exact and approximate projection approaches. Journal of Chemical Physics, 2019, 150, 184109.	1.2	46
86	Fast and Anomalous Exciton Diffusion in Two-Dimensional Hybrid Perovskites. Nano Letters, 2020, 20, 6674-6681.	4.5	44
87	The Electronic Structure of Mixed Self-Assembled Monolayers. ACS Nano, 2010, 4, 6735-6746.	7.3	43
88	On the accuracy of surface hopping dynamics in condensed phase non-adiabatic problems. Journal of Chemical Physics, 2016, 144, 094104.	1.2	43
89	Crossovers in the dynamics of supercooled liquids probed by an amorphous wall. Physical Review E, 2014, 89, 052311.	0.8	42
90	Molecular Engineering of Chromophores to Enable Tripletâ€“Triplet Annihilation Upconversion. Journal of the American Chemical Society, 2020, 142, 19917-19925.	6.6	42

#	Article	IF	Citations
91	Extending the applicability of Redfield theories into highly non-Markovian regimes. Journal of Chemical Physics, 2015, 143, 194108.	1.2	41
92	Impact of Anchoring Groups on Ballistic Transport: Single Molecule vs Monolayer Junctions. Journal of Physical Chemistry C, 2015, 119, 21198-21208.	1.5	40
93	Spatial extent of the excited exciton states in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>WS</mml:mi><mml:mn>2</mml:mn></mml:msub></m monolayers from diamagnetic shifts. Physical Review B, 2018, 98, .	3.7	40
94	Nonclassical Exciton Diffusion in Monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>WSe</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></ Physical Review Letters, 2021, 127, 076801.	2.9	40
95	Dielectric Engineering of Electronic Correlations in a van der Waals Heterostructure. Nano Letters, 2018, 18, 1402-1409.	4.5	39
96	Singletâ€“Triplet Energy Gaps of Organic Biradicals and Polyacenes with Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2019, 15, 4924-4932.	2.3	37
97	Attractive versus truncated repulsive supercooled liquids: The dynamics is encoded in the pair correlation function. Physical Review E, 2020, 101, 010602.	0.8	37
98	Quasi-1D exciton channels in strain-engineered 2D materials. Science Advances, 2021, 7, eabj3066.	4.7	37
99	Understanding Structure and Bonding of Multilayered Metalâ€“Organic Nanostructures. Journal of Physical Chemistry C, 2013, 117, 3055-3061.	1.5	36
100	Phaseless Auxiliary-Field Quantum Monte Carlo on Graphical Processing Units. Journal of Chemical Theory and Computation, 2018, 14, 4109-4121.	2.3	35
101	Multiset Matrix Product State Calculations Reveal Mobile Franck-Condon Excitations Under Strong Holstein-Type Coupling. Physical Review Letters, 2019, 123, 126601.	2.9	35
102	Many-body localization in system with a completely delocalized single-particle spectrum. Physical Review B, 2016, 94, .	1.1	34
103	Collectively Induced Quantum-Confined Stark Effect in Monolayers of Molecules Consisting of Polar Repeating Units. Journal of the American Chemical Society, 2011, 133, 18634-18645.	6.6	33
104	Anderson-Holstein model in two flavors of the noncrossing approximation. Physical Review B, 2016, 93, .	1.1	33
105	Inchworm Monte Carlo for exact non-adiabatic dynamics. II. Benchmarks and comparison with established methods. Journal of Chemical Physics, 2017, 146, 054106.	1.2	33
106	Chemical Transformations Approaching Chemical Accuracy via Correlated Sampling in Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2017, 13, 2667-2680.	2.3	33
107	Equilibrium ultrastable glasses produced by random pinning. Journal of Chemical Physics, 2014, 141, 224503.	1.2	31
108	Dipole-induced asymmetric conduction in tunneling junctions comprising self-assembled monolayers. RSC Advances, 2016, 6, 69479-69483.	1.7	31

#	Article	IF	Citations
109	Narrow-band high-lying excitonsÂwith negative-mass electrons in monolayer WSe2. Nature Communications, 2021, 12, 5500.	5.8	29
110	Self-assembled monolayers of polar molecules on Au(111) surfaces: distributing the dipoles. Physical Chemistry Chemical Physics, 2010, 12, 4291.	1.3	28
111	On the Role of Hydrodynamic Interactions in Colloidal Gelation. Journal of the Physical Society of Japan, 2008, 77, 084804.	0.7	27
112	Intermediate Bands in Zero-Dimensional Antimony Halide Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 4652-4656.	2.1	27
113	Relaxation patterns in supercooled liquids from generalized mode-coupling theory. Physical Review E, 2014, 90, 052306.	0.8	26
114	Autoionization and Dressing of Excited Excitons by Free Carriers in Monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>WSe</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:r Physical Review Letters, 2020, 125, 267401.	2.9	26
115	Resonant Cavity Modification of Ground-State Chemical Kinetics. Journal of Physical Chemistry Letters, 2022, 13, 6580-6586.	2.1	26
116	Finite-temperature auxiliary-field quantum Monte Carlo technique for Bose-Fermi mixtures. Physical Review A, 2012, 86, .	1.0	25
117	Effect of Moleculeâ€“Surface Reaction Mechanism on the Electronic Characteristics and Photovoltaic Performance of Molecularly Modified Si. Journal of Physical Chemistry C, 2013, 117, 22351-22361.	1.5	25
118	Anticorrelation between the Evolution of Molecular Dipole Moments and Induced Work Function Modifications. Journal of Physical Chemistry Letters, 2013, 4, 3521-3526.	2.1	25
119	Interplay of Collective Electrostatic Effects and Level Alignment Dictates the Tunneling Rates across Halogenated Aromatic Monolayer Junctions. Journal of Physical Chemistry Letters, 2019, 10, 4142-4147.	2.1	25
120	Approximate but accurate quantum dynamics from the Mori formalism. II. Equilibrium time correlation functions. Journal of Chemical Physics, 2017, 146, 084110.	1.2	24
121	Anharmonic Lattice Vibrations in Smallâ€Molecule Organic Semiconductors. Advanced Materials, 2020, 32, 1908028.	11.1	24
122	The effect of ionic composition on acoustic phonon speeds in hybrid perovskites from Brillouin spectroscopy and density functional theory. Journal of Materials Chemistry C, 2018, 6, 3861-3868.	2.7	23
123	Polarity Switching of Charge Transport and Thermoelectricity in Selfâ€Assembled Monolayer Devices. Advanced Materials, 2012, 24, 4403-4407.	11.1	22
124	Impact of Collective Electrostatic Effects on Charge Transport through Molecular Monolayers. Journal of Physical Chemistry C, 2014, 118, 22395-22401.	1.5	22
125	Breakdown of the Static Approximation for Free Carrier Screening of Excitons in Monolayer Semiconductors. Physica Status Solidi (B): Basic Research, 2018, 255, 1800216.	0.7	22
126	Phonon-induced disorder in dynamics of optically pumped metals from nonlinear electron-phonon coupling. Nature Communications, 2021, 12, 5803.	5.8	22

#	Article	IF	Citations
127	Quantum quench spectroscopy of a Luttinger liquid: Ultrarelativistic density wave dynamics due to fractionalization in anXXZchain. Physical Review B, 2011, 84, .	1.1	21
128	Predicting Ligand-Dissociation Energies of 3d Coordination Complexes with Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2020, 16, 3041-3054.	2.3	21
129	Anharmonic host-lattice dynamics enable fast ion conduction in superionic AgI. Physical Review Materials, 2020, 4, .	0.9	21
130	A Toolbox for Controlling the Energetics and Localization of Electronic States in Selfâ€Assembled Organic Monolayers. Advanced Science, 2015, 2, 1400016.	5.6	20
131	Electronic Properties of Biphenylthiolates on Au(111): The Impact of Coverage Revisited. Journal of Physical Chemistry C, 2015, 119, 7817-7825.	1.5	20
132	Temporal Evolution of Low-Temperature Phonon Sidebands in Transition Metal Dichalcogenides. ACS Photonics, 2020, 7, 2756-2764.	3.2	20
133	Elastoplasticity Mediates Dynamical Heterogeneity Below the Mode Coupling Temperature. Physical Review Letters, 2021, 127, 048002.	2.9	20
134	Dimensionality effects in the electronic structure of organic semiconductors consisting of polar repeat units. Organic Electronics, 2012, 13, 3165-3176.	1.4	19
135	Calculation of Metallocene Ionization Potentials via Auxiliary Field Quantum Monte Carlo: Toward Benchmark Quantum Chemistry for Transition Metals. Journal of Chemical Theory and Computation, 2022, 18, 2845-2862.	2.3	18
136	On the accuracy of the PadÃ©-resummed master equation approach to dissipative quantum dynamics. Journal of Chemical Physics, 2016, 144, 154106.	1.2	17
137	Classical glasses, black holes, and strange quantum liquids. Physical Review B, 2019, 100, .	1.1	17
138	The performance of phaseless auxiliary-field quantum Monte Carlo on the ground state electronic energy of benzene. Journal of Chemical Physics, 2020, 153, 126101.	1.2	17
139	A single atom change turns insulating saturated wires into molecular conductors. Nature Communications, 2021, 12, 3432.	5.8	16
140	Dark exciton-exciton annihilation in monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>WSe</mml:mi></mml:mrow><mml:mn>2</mml:mn> Physical Review B, 2021, 104, .	1.1	16
141	Analytic continuation average spectrum method for quantum liquids. Journal of Chemical Physics, 2009, 131, 054502.	1.2	15
142	Effect of a Coulombic dot-lead coupling on the dynamics of a quantum dot. Physical Review B, 2010, 81, .	1.1	15
143	Generalization of fewest-switches surface hopping for coherences. Journal of Chemical Physics, 2018, 148, 102309.	1.2	15
144	Interlayer Excitons in Transitionâ€Metal Dichalcogenide Heterobilayers. Physica Status Solidi (B): Basic Research, 2019, 256, 1900308.	0.7	15

#	Article	IF	Citations
145	Stochastic resolution-of-the-identity auxiliary-field quantum Monte Carlo: Scaling reduction without overhead. Journal of Chemical Physics, 2020, 153, 044131.	1.2	15
146	Microscopic model of the doping dependence of linewidths in monolayer transition metal dichalcogenides. Journal of Chemical Physics, 2020, 152, 194705.	1.2	15
147	Superatomic solid solutions. Nature Chemistry, 2021, 13, 607-613.	6.6	15
148	Electron recoil effect in electrically tunable <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:msub><mml:mi>Se</mml:mi><mml:mi><mml:r monolayers. Physical Review B, 2022, 105, .	1.1	14
149	Critical Dynamical Heterogeneities Close to Continuous Second-Order Glass Transitions. Physical Review Letters, 2014, 113, 245701.	2.9	13
150	On mean-field theories of dynamics in supercooled liquids. Journal of Chemical Physics, 2019, 151, 084503.	1.2	13
151	Transversal Halide Motion Intensifies Bandâ€Toâ€Band Transitions in Halide Perovskites. Advanced Science, 2022, 9, e2200706.	5.6	12
152	Probing the Disorder Inside the Cubic Unit Cell of Halide Perovskites from First-Principles. ACS Applied Materials & Interfaces, 2022, 14, 22973-22981.	4.0	12
153	Path integral approach to the Wigner representation of canonical density operators for discrete systems coupled to harmonic baths. Journal of Chemical Physics, 2017, 146, 024107.	1.2	11
154	Bond-Peierls polaron: Moderate mass enhancement and current-carrying ground state. Physical Review B, 2021, 104, .	1.1	11
155	Dynamics of liquids in the large-dimensional limit. Physical Review E, 2021, 104, 054606.	0.8	11
156	Interlayer excitons in MoSe₂/2D perovskite hybrid heterostructures â€“ the interplay between charge and energy transfer. Nanoscale, 2022, 14, 8085-8095.	2.8	11
157	Spectroscopic Study of Anisotropic Excitons in Single Crystal Hexacene. Journal of Physical Chemistry Letters, 2014, 5, 3632-3635.	2.1	10
158	Adsorption Behavior of Nonplanar Phthalocyanines: Competition of Different Adsorption Conformations. Journal of Physical Chemistry C, 2016, 120, 6869-6875.	1.5	10
159	Spectral Functions from Auxiliary-Field Quantum Monte Carlo without Analytic Continuation: The Extended Koopmansâ€™ Theorem Approach. Journal of Chemical Theory and Computation, 2021, 17, 3372-3387.	2.3	10
160	Numerically exact generalized Green's function cluster expansions for electron-phonon problems. Physical Review B, 2021, 104, .	1.1	10
161	Transport through a quantum dot with excitonic dot-lead coupling. Physical Review B, 2011, 83, .	1.1	9
162	Transport through a quantum dot with two parallel Luttinger liquid leads. Physical Review B, 2011, 83, .	1.1	9

#	Article	IF	Citations
163	Electronic structure of dipeptides in the gas-phase and as an adsorbed monolayer. Physical Chemistry Chemical Physics, 2018, 20, 6860-6867.	1.3	9
164	Lightâ€“matter coupling and non-equilibrium dynamics of exchange-split trions in monolayer WS2. Journal of Chemical Physics, 2020, 153, 034706.	1.2	9
165	Multiple Stable Isopreneâ€“Ozone Complexes Reveal Complex Entrance Channel Dynamics in the Isoprene + Ozone Reaction. Journal of the American Chemical Society, 2020, 142, 10806-10813.	6.6	9
166	Constrained-path auxiliary-field quantum Monte Carlo for coupled electrons and phonons. Physical Review B, 2021, 103, .	1.1	9
167	Vacancy control in acene blends links exothermic singlet fission to coherence. Nature Communications, 2021, 12, 5149.	5.8	9
168	Intermolecular coupling and superconductivity in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>PbMo</mml:mi><mml:mn>6</mml:mn></m mathvariant="normal">S</mml:mi><mml:mn>8</mml:mn></mml:msub></mml:mrow></mml:math> and other Chevrel phase compounds. Physical Review Materials, 2018, 2, .	0.9	9
169	Anharmonic Lattice Dynamics in Sodium Ion Conductors. Journal of Physical Chemistry Letters, 2022, 13, 5938-5945.	2.1	9
170	Tuning the Electronic Structure of Graphene through Collective Electrostatic Effects. Advanced Materials Interfaces, 2015, 2, 1500323.	1.9	8
171	Description of quasiparticle and satellite properties via cumulant expansions of the retarded one-particle Green's function. Physical Review B, 2016, 94, .	1.1	8
172	Accurate Molecular Geometries in Complex Excited-State Potential Energy Surfaces from Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 357-366.	2.3	8
173	Spectral asymmetry of phonon sideband luminescence in monolayer and bilayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>WSe</mml:mi><mml:mn>2</mml:mn></mml:msub></ Physical Review Research, 2021, 3, .	1.3	8
174	Relationship between two-level systems and quasilocalized normal modes in glasses. Physical Review Materials, 2021, 5, .	0.9	7
175	Revisiting the concept of activation in supercooled liquids. European Physical Journal E, 2021, 44, 77.	0.7	7
176	Time evolution of ML-MCTDH wavefunctions. I. Gauge conditions, basis functions, and singularities. Journal of Chemical Physics, 2021, 155, 174108.	1.2	7
177	A Localized-Orbital Energy Evaluation for Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2022, 18, 3447-3459.	2.3	7
178	Reorganization energy and polaronic effects of pentacene on NaCl films. Physical Review B, 2020, 102, .	1.1	6
179	Non-equilibrium diffusion of dark excitons in atomically thin semiconductors. Nanoscale, 2021, 13, 19966-19972.	2.8	6
180	On Stochastic Models of Dynamic Disorderâ€. Journal of Physical Chemistry B, 2006, 110, 19061-19065.	1.2	5

#	Article	IF	Citations
181	Time evolution of ML-MCTDH wavefunctions. II. Application of the projector splitting integrator. Journal of Chemical Physics, 2021, 155, 174109.	1.2	5
182	Assessing the accuracy of screened range-separated hybrids for bulk properties of semiconductors. Physical Review Materials, 2021, 5, .	0.9	4
183	Magnetic configurations of open-shell molecules on metals: The case of CuPc and CoPc on silver. Physical Review Materials, 2019, 3, .	0.9	4
184	Singlet fission. Journal of Chemical Physics, 2020, 153, 110401.	1.2	3
185	JCP Emerging Investigator Special Collection 2019. Journal of Chemical Physics, 2020, 153, 110402.	1.2	2
186	Breakdown of the Static Picture of Defect Energetics in Halide Perovskites: the Case of the Br Vacancy in CsPbBr3. , 0, , .		2
187	2D materials. Journal of Chemical Physics, 2021, 154, 040401.	1.2	1
188	Strongly Correlated Ladders in K-Doped p-Terphenyl Crystals. Nano Letters, 2021, 21, 9573-9579.	4.5	1
189	2020 JCP Emerging Investigator Special Collection. Journal of Chemical Physics, 2021, 155, 230401.	1.2	1
190	Chemical physics of materials. Journal of Chemical Physics, 2020, 153, 100402.	1.2	0
191	Optical Phonons in Halide Perovskites and Implications for Charge Transport. , 0, , .		0
192	Tuning the Tunnelling Decay Coefficient Using Single Polarizable Atoms via Energy Level Engineering of the Frontier Orbitals. , 0, , .		0
193	Role of Transversal Atomic Displacements in Halide Perovskites at Finite Temperature. , 0, , .		0
194	Tuning the Tunnelling Decay Coefficient Using Single Polarizable Atoms via Energy Level Engineering of the Frontier Orbitals. , 0, , .		0
195	Optical Phonons in Halide Perovskites and Implications for Charge Transport. , 0, , .		0
196	Sub-unit-cell disorder and intensified band-to-band transitions in halide perovskites from first-principles. , 0, , .		0