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	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, .	3.7	14
2	Unbiasing fermionic quantum Monte Carlo with a quantum computer. Nature, 2022, 603, 416-420.	13.7	84
3	Transversal Halide Motion Intensifies Bandâ€Toâ€Band Transitions in Halide Perovskites. Advanced Science, 2022, 9, e2200706.	5.6	12
4	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
5	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
6	Interlayer excitons in MoSe₂/2D perovskite hybrid heterostructures â€“ the interplay between charge and energy transfer. Nanoscale, 2022, 14, 8085-8095.	2.8	11
7	A Localized-Orbital Energy Evaluation for Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2022, 18, 3447-3459.	2.3	7
8	Anharmonic Lattice Dynamics in Sodium Ion Conductors. Journal of Physical Chemistry Letters, 2022, 13, 5938-5945.	2.1	9
9	Resonant Cavity Modification of Ground-State Chemical Kinetics. Journal of Physical Chemistry Letters, 2022, 13, 6580-6586.	2.1	26
10	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
11	2D materials. Journal of Chemical Physics, 2021, 154, 040401.	1.2	1
12	Constrained-path auxiliary-field quantum Monte Carlo for coupled electrons and phonons. Physical Review B, 2021, 103, .	1.1	9
13	Assessing the accuracy of screened range-separated hybrids for bulk properties of semiconductors. Physical Review Materials, 2021, 5, .	0.9	4
14	Superatomic solid solutions. Nature Chemistry, 2021, 13, 607-613.	6.6	15
15	Relationship between two-level systems and quasilocalized normal modes in glasses. Physical Review Materials, 2021, 5, .	0.9	7
16	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
17	The Significance of Polarons and Dynamic Disorder in Halide Perovskites. ACS Energy Letters, 2021, 6, 2162-2173.	8.8	74
18	A single atom change turns insulating saturated wires into molecular conductors. Nature Communications, 2021, 12, 3432.	5.8	16

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19	Revisiting the concept of activation in supercooled liquids. European Physical Journal E, 2021, 44, 77.	0.7	7
20	Elastoplasticity Mediates Dynamical Heterogeneity Below the Mode Coupling Temperature. Physical Review Letters, 2021, 127, 048002.	2.9	20
21	Numerically exact generalized Green's function cluster expansions for electron-phonon problems. Physical Review B, 2021, 104, .	1.1	10
22	Vacancy control in acene blends links exothermic singlet fission to coherence. Nature Communications, 2021, 12, 5149.	5.8	9
23	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
24	Narrow-band high-lying excitonsÂwith negative-mass electrons in monolayer WSe2. Nature Communications, 2021, 12, 5500.	5.8	29
25	Roadmap on organicâ€“inorganic hybrid perovskite semiconductors and devices. APL Materials, 2021, 9, .	2.2	102
26	Phonon-induced disorder in dynamics of optically pumped metals from nonlinear electron-phonon coupling. Nature Communications, 2021, 12, 5803.	5.8	22
27	Time evolution of ML-MCTDH wavefunctions. II. Application of the projector splitting integrator. Journal of Chemical Physics, 2021, 155, 174109.	1.2	5
28	Time evolution of ML-MCTDH wavefunctions. I. Gauge conditions, basis functions, and singularities. Journal of Chemical Physics, 2021, 155, 174108.	1.2	7
29	Quasi-1D exciton channels in strain-engineered 2D materials. Science Advances, 2021, 7, eabj3066.	4.7	37
30	Bond-Peierls polaron: Moderate mass enhancement and current-carrying ground state. Physical Review B, 2021, 104, .	1.1	11
31	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
32	Dynamics of liquids in the large-dimensional limit. Physical Review E, 2021, 104, 054606.	0.8	11
33	Strongly Correlated Ladders in K-Doped p-Terphenyl Crystals. Nano Letters, 2021, 21, 9573-9579.	4.5	1
34	Non-equilibrium diffusion of dark excitons in atomically thin semiconductors. Nanoscale, 2021, 13, 19966-19972.	2.8	6
35	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:mrow><mml:mn>2 Physical Review B, 2021, 104, .	1.1	10
36	2020 JCP Emerging Investigator Special Collection. Journal of Chemical Physics, 2021, 155, 230401.	1.2	1

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37	JCP Emerging Investigator Special Collection 2019. Journal of Chemical Physics, 2020, 153, 110402.	1.2	2
38	Lightâ€“matter coupling and non-equilibrium dynamics of exchange-split trions in monolayer WS2. Journal of Chemical Physics, 2020, 153, 034706.	1.2	9
39	Molecular Engineering of Chromophores to Enable Tripletâ€“Triplet Annihilation Upconversion. Journal of the American Chemical Society, 2020, 142, 19917-19925.	6.6	42
40	Fast and Anomalous Exciton Diffusion in Two-Dimensional Hybrid Perovskites. Nano Letters, 2020, 20, 6674-6681.	4.5	44
41	Broad Tunability of Carrier Effective Masses in Two-Dimensional Halide Perovskites. ACS Energy Letters, 2020, 5, 3609-3616.	8.8	54
42	Singlet fission. Journal of Chemical Physics, 2020, 153, 110401.	1.2	3
43	Reorganization energy and polaronic effects of pentacene on NaCl films. Physical Review B, 2020, 102, .	1.1	6
44	Chemical physics of materials. Journal of Chemical Physics, 2020, 153, 100402.	1.2	0
45	Temporal Evolution of Low-Temperature Phonon Sidebands in Transition Metal Dichalcogenides. ACS Photonics, 2020, 7, 2756-2764.	3.2	20
46	Stochastic resolution-of-the-identity auxiliary-field quantum Monte Carlo: Scaling reduction without overhead. Journal of Chemical Physics, 2020, 153, 044131.	1.2	15
47	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
48	Depletion of Two-Level Systems in Ultrastable Computer-Generated Glasses. Physical Review Letters, 2020, 124, 225901.	2.9	47
49	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
50	Microscopic model of the doping dependence of linewidths in monolayer transition metal dichalcogenides. Journal of Chemical Physics, 2020, 152, 194705.	1.2	15
51	Exciton diffusion in monolayer semiconductors with suppressed disorder. Physical Review B, 2020, 101, .	1.1	74
52	Attractive versus truncated repulsive supercooled liquids: The dynamics is encoded in the pair correlation function. Physical Review E, 2020, 101, 010602.	0.8	37
53	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
54	Anharmonic Lattice Vibrations in Smallâ€Molecule Organic Semiconductors. Advanced Materials, 2020, 32, 1908028.	11.1	24

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55	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> Physical Review Letters, 2020, 125, 267401.	2.9	26
56	Anharmonic host-lattice dynamics enable fast ion conduction in superionic AgI. Physical Review Materials, 2020, 4, .	0.9	21
57	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
58	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
59	Dielectric disorder in two-dimensional materials. Nature Nanotechnology, 2019, 14, 832-837.	15.6	223
60	Dynamic shortening of disorder potentials in anharmonic halide perovskites. Nature Communications, 2019, 10, 3141.	5.8	74
61	Removing instabilities in the hierarchical equations of motion: Exact and approximate projection approaches. Journal of Chemical Physics, 2019, 150, 184109.	1.2	46
62	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
63	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
64	Interlayer Excitons in Transitionâ€Metal Dichalcogenide Heterobilayers. Physica Status Solidi (B): Basic Research, 2019, 256, 1900308.	0.7	15
65	Exciton Propagation and Halo Formation in Two-Dimensional Materials. Nano Letters, 2019, 19, 7317-7323.	4.5	64
66	Multiset Matrix Product State Calculations Reveal Mobile Franck-Condon Excitations Under Strong Holstein-Type Coupling. Physical Review Letters, 2019, 123, 126601.	2.9	35
67	On mean-field theories of dynamics in supercooled liquids. Journal of Chemical Physics, 2019, 151, 084503.	1.2	13
68	Intrinsic lifetime of higher excitonic states in tungsten diselenide monolayers. Nanoscale, 2019, 11, 12381-12387.	2.8	56
69	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
70	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
71	Length- and Thickness-Dependent Optical Response of Liquid-Exfoliated Transition Metal Dichalcogenides. Chemistry of Materials, 2019, 31, 10049-10062.	3.2	57
72	Classical glasses, black holes, and strange quantum liquids. Physical Review B, 2019, 100, .	1.1	17

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73	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
74	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:m plus Bethe-Salpeter approach. Physical Review Materials, 2019, 3, .	0.9	61
75	Magnetic configurations of open-shell molecules on metals: The case of CuPc and CoPc on silver. Physical Review Materials, 2019, 3, .	0.9	4
76	Colloquium : Excitons in atomically thin transition metal dichalcogenides. Reviews of Modern Physics, 2018, 90, .	16.4	1,292
77	Electronic structure of dipeptides in the gas-phase and as an adsorbed monolayer. Physical Chemistry Chemical Physics, 2018, 20, 6860-6867.	1.3	9
78	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
79	Dielectric Engineering of Electronic Correlations in a van der Waals Heterostructure. Nano Letters, 2018, 18, 1402-1409.	4.5	39
80	Optical and Excitonic Properties of Atomically Thin Transition-Metal Dichalcogenides. Annual Review of Condensed Matter Physics, 2018, 9, 379-396.	5.2	68
81	Generalization of fewest-switches surface hopping for coherences. Journal of Chemical Physics, 2018, 148, 102309.	1.2	15
82	Momentum-space indirect interlayer excitons in transition-metal dichalcogenide van der Waals heterostructures. Nature Physics, 2018, 14, 801-805.	6.5	229
83	What Remains Unexplained about the Properties of Halide Perovskites?. Advanced Materials, 2018, 30, e1800691.	11.1	231
84	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
85	How Lattice and Charge Fluctuations Control Carrier Dynamics in Halide Perovskites. Nano Letters, 2018, 18, 8041-8046.	4.5	97
86	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></mm monolayers from diamagnetic shifts. Physical Review B, 2018, 98, .	3.7	40
87	Exciton Diffusion and Halo Effects in Monolayer Semiconductors. Physical Review Letters, 2018, 120, 207401.	2.9	193
88	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:mrow></m Physical Review Letters, 2018, 121, 057402.	2.9	70
89	Intermediate Bands in Zero-Dimensional Antimony Halide Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 4652-4656.	2.1	27
90	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

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91	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
92	Enhancement of Excitonâ€“Phonon Scattering from Monolayer to Bilayer WS₂. Nano Letters, 2018, 18, 6135-6143.	4.5	50
93	Phaseless Auxiliary-Field Quantum Monte Carlo on Graphical Processing Units. Journal of Chemical Theory and Computation, 2018, 14, 4109-4121.	2.3	35
94	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
95	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
96	Transient superconductivity from electronic squeezing of optically pumped phonons. Nature Physics, 2017, 13, 479-483.	6.5	139
97	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
98	Inchworm Monte Carlo for exact non-adiabatic dynamics. I. Theory and algorithms. Journal of Chemical Physics, 2017, 146, 054105.	1.2	47
99	Direct Observation of Ultrafast Exciton Formation in a Monolayer of WSe₂. Nano Letters, 2017, 17, 1455-1460.	4.5	171
100	Approximate but accurate quantum dynamics from the Mori formalism. II. Equilibrium time correlation functions. Journal of Chemical Physics, 2017, 146, 084110.	1.2	24
101	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
102	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
103	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
104	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
105	Coulomb engineering of the bandgap and excitons in two-dimensional materials. Nature Communications, 2017, 8, 15251.	5.8	526
106	Local Polar Fluctuations in Lead Halide Perovskite Crystals. Physical Review Letters, 2017, 118, 136001.	2.9	489
107	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></m /graphene heterostructures. Physical Review B, 2017, 96, .	3.7	46
108	Light-induced picosecond rotational disordering of the inorganic sublattice in hybrid perovskites. Science Advances, 2017, 3, e1602388.	4.7	149

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109	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
110	Single-crystal-to-single-crystal intercalation of a low-bandgap superatomic crystal. Nature Chemistry, 2017, 9, 1170-1174.	6.6	56
111	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
112	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
113	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
114	On the accuracy of surface hopping dynamics in condensed phase non-adiabatic problems. Journal of Chemical Physics, 2016, 144, 094104.	1.2	43
115	On the accuracy of the PadÃ©-resummed master equation approach to dissipative quantum dynamics. Journal of Chemical Physics, 2016, 144, 154106.	1.2	17
116	Approximate but accurate quantum dynamics from the Mori formalism: I. Nonequilibrium dynamics. Journal of Chemical Physics, 2016, 144, 184104.	1.2	48
117	High Chloride Doping Levels Stabilize the Perovskite Phase of Cesium Lead Iodide. Nano Letters, 2016, 16, 3563-3570.	4.5	247
118	Optical phonons in methylammonium lead halide perovskites and implications for charge transport. Materials Horizons, 2016, 3, 613-620.	6.4	299
119	Many-body localization in system with a completely delocalized single-particle spectrum. Physical Review B, 2016, 94, .	1.1	34
120	Anderson-Holstein model in two flavors of the noncrossing approximation. Physical Review B, 2016, 93, .	1.1	33
121	Dipole-induced asymmetric conduction in tunneling junctions comprising self-assembled monolayers. RSC Advances, 2016, 6, 69479-69483.	1.7	31
122	Excitonic linewidth and coherence lifetime in monolayer transition metal dichalcogenides. Nature Communications, 2016, 7, 13279.	5.8	360
123	Hybrid organicâ€”inorganic perovskites: low-cost semiconductors with intriguing charge-transport properties. Nature Reviews Materials, 2016, 1, .	23.3	1,173
124	Hybrid Organicâ€“Inorganic Perovskites on the Move. Accounts of Chemical Research, 2016, 49, 573-581.	7.6	227
125	Adsorption Behavior of Nonplanar Phthalocyanines: Competition of Different Adsorption Conformations. Journal of Physical Chemistry C, 2016, 120, 6869-6875.	1.5	10
126	Transition voltages respond to synthetic reorientation of embedded dipoles in self-assembled monolayers. Chemical Science, 2016, 7, 781-787.	3.7	46

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127	Bright and dark singlet excitons via linear and two-photon spectroscopy in monolayer transition-metal dichalcogenides. Physical Review B, 2015, 92, .	1.1	68
128	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
129	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><mml:mn>Physical Review Letters, 2015, 115, 126802.	2.9	323
130	Microscopic Dynamics of Supercooled Liquids from First Principles. Physical Review Letters, 2015, 115, 205701.	2.9	62
131	Taming the Dynamical Sign Problem in Real-Time Evolution of Quantum Many-Body Problems. Physical Review Letters, 2015, 115, 266802.	2.9	138
132	Extending the applicability of Redfield theories into highly non-Markovian regimes. Journal of Chemical Physics, 2015, 143, 194108.	1.2	41
133	Hybrid Organicâ€“Inorganic Perovskites (HOIPs): Opportunities and Challenges. Advanced Materials, 2015, 27, 5102-5112.	11.1	372
134	The Effects of Embedded Dipoles in Aromatic Selfâ€Assembled Monolayers. Advanced Functional Materials, 2015, 25, 3943-3957.	7.8	90
135	Theory of Hydrogen Migration in Organicâ€“Inorganic Halide Perovskites. Angewandte Chemie - International Edition, 2015, 54, 12437-12441.	7.2	134
136	Tuning the Electronic Structure of Graphene through Collective Electrostatic Effects. Advanced Materials Interfaces, 2015, 2, 1500323.	1.9	8
137	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
138	A Toolbox for Controlling the Energetics and Localization of Electronic States in Selfâ€Assembled Organic Monolayers. Advanced Science, 2015, 2, 1400016.	5.6	20
139	Perovskite Solar Cells: Do We Know What We Do Not Know?. Journal of Physical Chemistry Letters, 2015, 6, 279-282.	2.1	71
140	Population inversion and giant bandgap renormalization in atomically thin WS2 layers. Nature Photonics, 2015, 9, 466-470.	15.6	366
141	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
142	Excitons in ultrathin organic-inorganic perovskite crystals. Physical Review B, 2015, 92, .	1.1	263
143	Reliable Energy Level Alignment at Physisorbed Moleculeâ€“Metal Interfaces from Density Functional Theory. Nano Letters, 2015, 15, 2448-2455.	4.5	112
144	Electronic Properties of Biphenylthiolates on Au(111): The Impact of Coverage Revisited. Journal of Physical Chemistry C, 2015, 119, 7817-7825.	1.5	20

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145	Observation of biexcitons in monolayer WSe2. Nature Physics, 2015, 11, 477-481.	6.5	531
146	Impact of Anchoring Groups on Ballistic Transport: Single Molecule vs Monolayer Junctions. Journal of Physical Chemistry C, 2015, 119, 21198-21208.	1.5	40
147	Are Mobilities in Hybrid Organicâ€“Inorganic Halide Perovskites Actually â€œHighâ€?. Journal of Physical Chemistry Letters, 2015, 6, 4754-4757.	2.1	197
148	Relaxation patterns in supercooled liquids from generalized mode-coupling theory. Physical Review E, 2014, 90, 052306.	0.8	26
149	Critical Dynamical Heterogeneities Close to Continuous Second-Order Glass Transitions. Physical Review Letters, 2014, 113, 245701.	2.9	13
150	Equilibrium ultrastable glasses produced by random pinning. Journal of Chemical Physics, 2014, 141, 224503.	1.2	31
151	Microscopic theory of singlet exciton fission. III. Crystalline pentacene. Journal of Chemical Physics, 2014, 141, 074705.	1.2	160
152	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	1.1	1,017
153	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
154	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
155	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
156	Correlation of Local Order with Particle Mobility in Supercooled Liquids Is Highly System Dependent. Physical Review Letters, 2014, 113, 157801.	2.9	83
157	Impact of Collective Electrostatic Effects on Charge Transport through Molecular Monolayers. Journal of Physical Chemistry C, 2014, 118, 22395-22401.	1.5	22
158	Spectroscopic Study of Anisotropic Excitons in Single Crystal Hexacene. Journal of Physical Chemistry Letters, 2014, 5, 3632-3635.	2.1	10
159	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
160	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></mml:mrow><mml:mn> Physical Review Letters, 2014, 113, 076802.	2.9	1,814
161	Crossovers in the dynamics of supercooled liquids probed by an amorphous wall. Physical Review E, 2014, 89, 052311.	0.8	42
162	Green's functions from real-time bold-line Monte Carlo. Physical Review B, 2014, 89, .	1.1	51

#	Article	IF	Citations
163	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
164	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
165	Theory of neutral and charged excitons in monolayer transition metal dichalcogenides. Physical Review B, 2013, 88, .	1.1	737
166	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
167	The Quantum Coherent Mechanism for Singlet Fission: Experiment and Theory. Accounts of Chemical Research, 2013, 46, 1321-1329.	7.6	262
168	Understanding Structure and Bonding of Multilayered Metalâ€“Organic Nanostructures. Journal of Physical Chemistry C, 2013, 117, 3055-3061.	1.5	36
169	Numerically exact long-time magnetization dynamics at the nonequilibrium Kondo crossover of the Anderson impurity model. Physical Review B, 2013, 87, .	1.1	111
170	Accurate Force Field Development for Modeling Conjugated Polymers. Journal of Chemical Theory and Computation, 2012, 8, 4556-4569.	2.3	109
171	Finite-temperature auxiliary-field quantum Monte Carlo technique for Bose-Fermi mixtures. Physical Review A, 2012, 86, .	1.0	25
172	Dimensionality effects in the electronic structure of organic semiconductors consisting of polar repeat units. Organic Electronics, 2012, 13, 3165-3176.	1.4	19
173	Polarity Switching of Charge Transport and Thermoelectricity in Selfâ€Assembled Monolayer Devices. Advanced Materials, 2012, 24, 4403-4407.	11.1	22
174	Quantum quench spectroscopy of a Luttinger liquid: Ultrarelativistic density wave dynamics due to fractionalization in anXXZchain. Physical Review B, 2011, 84, .	1.1	21
175	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
176	Quantum fluctuations can promote or inhibit glassÂformation. Nature Physics, 2011, 7, 134-137.	6.5	84
177	Numerically exact long-time behavior of nonequilibrium quantum impurity models. Physical Review B, 2011, 84, .	1.1	55
178	Transport through a quantum dot with excitonic dot-lead coupling. Physical Review B, 2011, 83, .	1.1	9
179	Transport through a quantum dot with two parallel Luttinger liquid leads. Physical Review B, 2011, 83, .	1.1	9
180	Effect of a Coulombic dot-lead coupling on the dynamics of a quantum dot. Physical Review B, 2010, 81, .	1.1	15

#	Article	IF	Citations
181	Bold-line diagrammatic Monte Carlo method: General formulation and application to expansion around the noncrossing approximation. Physical Review B, 2010, 82, .	1.1	64
182	Work-Function Modification beyond Pinning: When Do Molecular Dipoles Count?. Nano Letters, 2010, 10, 4369-4374.	4.5	70
183	The Electronic Structure of Mixed Self-Assembled Monolayers. ACS Nano, 2010, 4, 6735-6746.	7.3	43
184	Self-assembled monolayers of polar molecules on Au(111) surfaces: distributing the dipoles. Physical Chemistry Chemical Physics, 2010, 12, 4291.	1.3	28
185	Analytic continuation average spectrum method for quantum liquids. Journal of Chemical Physics, 2009, 131, 054502.	1.2	15
186	Irreversible reorganization in a supercooled liquid originates from localized soft modes. Nature Physics, 2008, 4, 711-715.	6.5	367
187	On the Role of Hydrodynamic Interactions in Colloidal Gelation. Journal of the Physical Society of Japan, 2008, 77, 084804.	0.7	27
188	On Stochastic Models of Dynamic Disorderâ€. Journal of Physical Chemistry B, 2006, 110, 19061-19065.	1.2	5
189	Comparison of Dynamical Heterogeneity in Hard-Sphere and Attractive Glass Formersâ€. Journal of Physical Chemistry B, 2005, 109, 14654-14658.	1.2	49
190	Optical Phonons in Halide Perovskites and Implications for Charge Transport. , 0, , .		0
191	Tuning the Tunnelling Decay Coefficient Using Single Polarizable Atoms via Energy Level Engineering of the Frontier Orbitals. , 0, , .		0
192	Role of Transversal Atomic Displacements in Halide Perovskites at Finite Temperature. , 0, , .		0
193	Tuning the Tunnelling Decay Coefficient Using Single Polarizable Atoms via Energy Level Engineering of the Frontier Orbitals. , 0, , .		0
194	Optical Phonons in Halide Perovskites and Implications for Charge Transport. , 0, , .		0
195	Breakdown of the Static Picture of Defect Energetics in Halide Perovskites: the Case of the Br Vacancy in CsPbBr3. , 0, , .		2
196	Sub-unit-cell disorder and intensified band-to-band transitions in halide perovskites from first-principles. , 0, , .		0