David A Egger

List of Publications by Year in Descending Order

174 papers	14,281 citations	55 h-index	117 g-index
198 ext. papers	17,174 ext. citations	8.6 avg, IF	7.03 L-index

#	Paper	IF	Citations
174	Unbiasing fermionic quantum Monte Carlo with a quantum computer.. *Nature*, **2022**, 603, 416-420	50.4	10
173	Transversal Halide Motion Intensifies Band-To-Band Transitions in Halide Perovskites.. *Advanced Science*, **2022**, e2200706	13.6	2
172	Spectral asymmetry of phonon sideband luminescence in monolayer and bilayer WSe2. *Physical Review Research*, **2021**, 3,	3.9	3
171	Dynamics of liquids in the large-dimensional limit.. *Physical Review E*, **2021**, 104, 054606	2.4	3
170	Strongly Correlated Ladders in K-Doped -Terphenyl Crystals. *Nano Letters*, **2021**, 21, 9573-9579	11.5	
169	Phonon-induced disorder in dynamics of optically pumped metals from nonlinear electron-phonon coupling. *Nature Communications*, **2021**, 12, 5803	17.4	3
168	Time evolution of ML-MCTDH wavefunctions. II. Application of the projector splitting integrator. *Journal of Chemical Physics*, **2021**, 155, 174109	3.9	1
167	Time evolution of ML-MCTDH wavefunctions. I. Gauge conditions, basis functions, and singularities. *Journal of Chemical Physics*, **2021**, 155, 174108	3.9	2
166	Quasi-1D exciton channels in strain-engineered 2D materials. *Science Advances*, **2021**, 7, eabj3066	14.3	6
165	Roadmap on organic–inorganic hybrid perovskite semiconductors and devices. *APL Materials*, **2021**, 9, 109202	5.7	28
164	Constrained-path auxiliary-field quantum Monte Carlo for coupled electrons and phonons. *Physical Review B*, **2021**, 103,	3.3	3
163	Assessing the accuracy of screened range-separated hybrids for bulk properties of semiconductors. *Physical Review Materials*, **2021**, 5,	3.2	1
162	Superatomic solid solutions. *Nature Chemistry*, **2021**, 13, 607-613	17.6	4
161	Relationship between two-level systems and quasilocalized normal modes in glasses. *Physical Review Materials*, **2021**, 5,	3.2	3
160	Spectral Functions from Auxiliary-Field Quantum Monte Carlo without Analytic Continuation: The Extended Koopmans’ Theorem Approach. *Journal of Chemical Theory and Computation*, **2021**, 17, 3372-3387	6.4	5
159	The Significance of Polarons and Dynamic Disorder in Halide Perovskites. *ACS Energy Letters*, **2021**, 6, 2162-2173	20.1	17
158	A single atom change turns insulating saturated wires into molecular conductors. *Nature Communications*, **2021**, 12, 3432	17.4	5

157	Revisiting the concept of activation in supercooled liquids. *European Physical Journal E*, **2021**, 44, 77	1.5	2
156	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	6.4	1
155	Elastoplasticity Mediates Dynamical Heterogeneity Below the Mode Coupling Temperature. *Physical Review Letters*, **2021**, 127, 048002	7.4	3
154	Vacancy control in acene blends links exothermic singlet fission to coherence. *Nature Communications*, **2021**, 12, 5149	17.4	2
153	Nonclassical Exciton Diffusion in Monolayer WSe_{2}. *Physical Review Letters*, **2021**, 127, 076801	7.4	11
152	Narrow-band high-lying excitons´with negative-mass electrons in monolayer WSe. *Nature Communications*, **2021**, 12, 5500	17.4	5
151	Dark exciton-exciton annihilation in monolayer WSe2. *Physical Review B*, **2021**, 104,	3.3	3
150	Stochastic resolution-of-the-identity auxiliary-field quantum Monte Carlo: Scaling reduction without overhead. *Journal of Chemical Physics*, **2020**, 153, 044131	3.9	8
149	The performance of phaseless auxiliary-field quantum Monte Carlo on the ground state electronic energy of benzene. *Journal of Chemical Physics*, **2020**, 153, 126101	3.9	9
148	Depletion of Two-Level Systems in Ultrastable Computer-Generated Glasses. *Physical Review Letters*, **2020**, 124, 225901	7.4	20
147	Multiple Stable Isoprene-Ozone Complexes Reveal Complex Entrance Channel Dynamics in the Isoprene + Ozone Reaction. *Journal of the American Chemical Society*, **2020**, 142, 10806-10813	16.4	7
146	Microscopic model of the doping dependence of linewidths in monolayer transition metal dichalcogenides. *Journal of Chemical Physics*, **2020**, 152, 194705	3.9	8
145	Exciton diffusion in monolayer semiconductors with suppressed disorder. *Physical Review B*, **2020**, 101,	3.3	44
144	Attractive versus truncated repulsive supercooled liquids: The dynamics is encoded in the pair correlation function. *Physical Review E*, **2020**, 101, 010602	2.4	25
143	Autoionization and Dressing of Excited Excitons by Free Carriers in Monolayer WSe_{2}. *Physical Review Letters*, **2020**, 125, 267401	7.4	8
142	Anharmonic host-lattice dynamics enable fast ion conduction in superionic AgI. *Physical Review Materials*, **2020**, 4,	3.2	9
141	Light-matter coupling and non-equilibrium dynamics of exchange-split trions in monolayer WS. *Journal of Chemical Physics*, **2020**, 153, 034706	3.9	0
140	Molecular Engineering of Chromophores to Enable Triplet-Triplet Annihilation Upconversion. *Journal of the American Chemical Society*, **2020**, 142, 19917-19925	16.4	13

139	Fast and Anomalous Exciton Diffusion in Two-Dimensional Hybrid Perovskites. *Nano Letters*, **2020**, 20, 6674-6681	11.5	21
138	Broad Tunability of Carrier Effective Masses in Two-Dimensional Halide Perovskites. *ACS Energy Letters*, **2020**, 5, 3609-3616	20.1	22
137	Reorganization energy and polaronic effects of pentacene on NaCl films. *Physical Review B*, **2020**, 102,	3.3	4
136	Temporal Evolution of Low-Temperature Phonon Sidebands in Transition Metal Dichalcogenides. *ACS Photonics*, **2020**, 7, 2756-2764	6.3	9
135	Predicting Ligand-Dissociation Energies of 3d Coordination Complexes with Auxiliary-Field Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, **2020**, 16, 3041-3054	6.4	10
134	Anharmonic Lattice Vibrations in Small-Molecule Organic Semiconductors. *Advanced Materials*, **2020**, 32, e1908028	24	11
133	Exciton Propagation and Halo Formation in Two-Dimensional Materials. *Nano Letters*, **2019**, 19, 7317-7323	11.5	37
132	Multiset Matrix Product State Calculations Reveal Mobile Franck-Condon Excitations Under Strong Holstein-Type Coupling. *Physical Review Letters*, **2019**, 123, 126601	7.4	21
131	On mean-field theories of dynamics in supercooled liquids. *Journal of Chemical Physics*, **2019**, 151, 084503	3.9	9
130	Intrinsic lifetime of higher excitonic states in tungsten diselenide monolayers. *Nanoscale*, **2019**, 11, 12381-12387	7.7	40
129	On Achieving High Accuracy in Quantum Chemical Calculations of 3 d 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	6.4	42
128	Dynamic emission Stokes shift and liquid-like dielectric solvation of band edge carriers in lead-halide perovskites. *Nature Communications*, **2019**, 10, 1175	17.4	68
127	Singlet-Triplet Energy Gaps of Organic Biradicals and Polyacenes with Auxiliary-Field Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, **2019**, 15, 4924-4932	6.4	22
126	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	3.8	43
125	Dielectric disorder in two-dimensional materials. *Nature Nanotechnology*, **2019**, 14, 832-837	28.7	125
124	Dynamic shortening of disorder potentials in anharmonic halide perovskites. *Nature Communications*, **2019**, 10, 3141	17.4	35
123	Removing instabilities in the hierarchical equations of motion: Exact and approximate projection approaches. *Journal of Chemical Physics*, **2019**, 150, 184109	3.9	26
122	Breakdown of the Static Picture of Defect Energetics in Halide Perovskites: The Case of the Br Vacancy in CsPbBr. *Journal of Physical Chemistry Letters*, **2019**, 10, 4490-4498	6.4	25

121	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	6.4	20
120	Interlayer Excitons in Transition-Metal Dichalcogenide Heterobilayers. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1900308	1.3	7
119	Comparing time-dependent density functional theory with many-body perturbation theory for semiconductors: Screened range-separated hybrids and the GW plus Bethe-Salpeter approach. *Physical Review Materials*, **2019**, 3,	3.2	36
118	Magnetic configurations of open-shell molecules on metals: The case of CuPc and CoPc on silver. *Physical Review Materials*, **2019**, 3,	3.2	2
117	Length- and Thickness-Dependent Optical Response of Liquid-Exfoliated Transition Metal Dichalcogenides. *Chemistry of Materials*, **2019**, 31, 10049-10062	9.6	27
116	Classical glasses, black holes, and strange quantum liquids. *Physical Review B*, **2019**, 100,	3.3	9
115	Constructing the Electronic Structure of CHNHPbI and CHNHPbBr Perovskite Thin Films from Single-Crystal Band Structure Measurements. *Journal of Physical Chemistry Letters*, **2019**, 10, 601-609	6.4	55
114	Colloquium: Excitons in atomically thin transition metal dichalcogenides. *Reviews of Modern Physics*, **2018**, 90,	40.5	766
113	Electronic structure of dipeptides in the gas-phase and as an adsorbed monolayer. *Physical Chemistry Chemical Physics*, **2018**, 20, 6860-6867	3.6	8
112	Impact of Small Phonon Energies on the Charge-Carrier Lifetimes in Metal-Halide Perovskites. *Journal of Physical Chemistry Letters*, **2018**, 9, 939-946	6.4	66
111	Dielectric Engineering of Electronic Correlations in a van der Waals Heterostructure. *Nano Letters*, **2018**, 18, 1402-1409	11.5	32
110	Optical and Excitonic Properties of Atomically Thin Transition-Metal Dichalcogenides. *Annual Review of Condensed Matter Physics*, **2018**, 9, 379-396	19.7	46
109	Generalization of fewest-switches surface hopping for coherences. *Journal of Chemical Physics*, **2018**, 148, 102309	3.9	10
108	Momentum-space indirect interlayer excitons in transition-metal dichalcogenide van der Waals heterostructures. *Nature Physics*, **2018**, 14, 801-805	16.2	145
107	What Remains Unexplained about the Properties of Halide Perovskites?. *Advanced Materials*, **2018**, 30, e1800691	24	174
106	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	7.1	17
105	Zeeman Splitting and Inverted Polarization of Biexciton Emission in Monolayer WS_{2}. *Physical Review Letters*, **2018**, 121, 057402	7.4	48
104	Intermediate Bands in Zero-Dimensional Antimony Halide Perovskites. *Journal of Physical Chemistry Letters*, **2018**, 9, 4652-4656	6.4	22

103	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	3.9	55
102	Breakdown of the Static Approximation for Free Carrier Screening of Excitons in Monolayer Semiconductors. *Physica Status Solidi (B): Basic Research*, **2018**, 255, 1800216	1.3	14
101	Enhancement of Exciton-Phonon Scattering from Monolayer to Bilayer WS. *Nano Letters*, **2018**, 18, 6135-6143	11.5	27
100	Phaseless Auxiliary-Field Quantum Monte Carlo on Graphical Processing Units. *Journal of Chemical Theory and Computation*, **2018**, 14, 4109-4121	6.4	25
99	Intermolecular coupling and superconductivity in PbMo6S8 and other Chevrel phase compounds. *Physical Review Materials*, **2018**, 2,	3.2	7
98	How Lattice and Charge Fluctuations Control Carrier Dynamics in Halide Perovskites. *Nano Letters*, **2018**, 18, 8041-8046	11.5	51
97	Spatial extent of the excited exciton states in WS2 monolayers from diamagnetic shifts. *Physical Review B*, **2018**, 98,	3.3	23
96	Exciton Diffusion and Halo Effects in Monolayer Semiconductors. *Physical Review Letters*, **2018**, 120, 207401	7.4	116
95	The Role of Electronic and Phononic Excitation in the Optical Response of Monolayer WS after Ultrafast Excitation. *Nano Letters*, **2017**, 17, 644-651	11.5	106
94	Transient superconductivity from electronic squeezing of optically pumped phonons. *Nature Physics*, **2017**, 13, 479-483	16.2	104
93	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	3.9	10
92	Inchworm Monte Carlo for exact non-adiabatic dynamics. I. Theory and algorithms. *Journal of Chemical Physics*, **2017**, 146, 054105	3.9	32
91	Direct Observation of Ultrafast Exciton Formation in a Monolayer of WSe. *Nano Letters*, **2017**, 17, 1455-1460	11.5	126
90	Approximate but accurate quantum dynamics from the Mori formalism. II. Equilibrium time correlation functions. *Journal of Chemical Physics*, **2017**, 146, 084110	3.9	20
89	Inchworm Monte Carlo for exact non-adiabatic dynamics. II. Benchmarks and comparison with established methods. *Journal of Chemical Physics*, **2017**, 146, 054106	3.9	23
88	Vibronic exciton theory of singlet fission. II. Two-dimensional spectroscopic detection of the correlated triplet pair state. *Journal of Chemical Physics*, **2017**, 146, 174704	3.9	45
87	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	3.9	67
86	Chemical Transformations Approaching Chemical Accuracy via Correlated Sampling in Auxiliary-Field Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, **2017**, 13, 2667-2680	6.4	21

85	Coulomb engineering of the bandgap and excitons in two-dimensional materials. *Nature Communications*, **2017**, 8, 15251	17.4	334
84	Local Polar Fluctuations in Lead Halide Perovskite Crystals. *Physical Review Letters*, **2017**, 118, 136001	7.4	374
83	Exciton broadening in WS2/graphene heterostructures. *Physical Review B*, **2017**, 96,	3.3	38
82	Light-induced picosecond rotational disordering of the inorganic sublattice in hybrid perovskites. *Science Advances*, **2017**, 3, e1602388	14.3	109
81	Triplet Separation Drives Singlet Fission after Femtosecond Correlated Triplet Pair Production in Rubrene. *Journal of the American Chemical Society*, **2017**, 139, 11745-11751	16.4	85
80	Single-crystal-to-single-crystal intercalation of a low-bandgap superatomic crystal. *Nature Chemistry* , **2017**, 9, 1170-1174	17.6	44
79	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	6.4	55
78	Many-body localization in system with a completely delocalized single-particle spectrum. *Physical Review B*, **2016**, 94,	3.3	26
77	Anderson-Holstein model in two flavors of the noncrossing approximation. *Physical Review B*, **2016**, 93,	3.3	29
76	Dipole-induced asymmetric conduction in tunneling junctions comprising self-assembled monolayers. *RSC Advances*, **2016**, 6, 69479-69483	3.7	26
75	Excitonic linewidth and coherence lifetime in monolayer transition metal dichalcogenides. *Nature Communications*, **2016**, 7, 13279	17.4	248
74	Hybrid organic□inorganic perovskites: low-cost semiconductors with intriguing charge-transport properties. *Nature Reviews Materials*, **2016**, 1,	73.3	912
73	Hybrid Organic-Inorganic Perovskites on the Move. *Accounts of Chemical Research*, **2016**, 49, 573-81	24.3	176
72	Adsorption Behavior of Nonplanar Phthalocyanines: Competition of Different Adsorption Conformations. *Journal of Physical Chemistry C*, **2016**, 120, 6869-6875	3.8	9
71	Transition voltages respond to synthetic reorientation of embedded dipoles in self-assembled monolayers. *Chemical Science*, **2016**, 7, 781-787	9.4	33
70	Valence and Conduction Band Densities of States of Metal Halide Perovskites: A Combined Experimental-Theoretical Study. *Journal of Physical Chemistry Letters*, **2016**, 7, 2722-9	6.4	264
69	Description of quasiparticle and satellite properties via cumulant expansions of the retarded one-particle Green□ function. *Physical Review B*, **2016**, 94,	3.3	6
68	On the accuracy of surface hopping dynamics in condensed phase non-adiabatic problems. *Journal of Chemical Physics*, **2016**, 144, 094104	3.9	35

67	On the accuracy of the Pad□esummed master equation approach to dissipative quantum dynamics. *Journal of Chemical Physics*, **2016**, 144, 154106	3.9	15
66	Approximate but accurate quantum dynamics from the Mori formalism: I. Nonequilibrium dynamics. *Journal of Chemical Physics*, **2016**, 144, 184104	3.9	40
65	High Chloride Doping Levels Stabilize the Perovskite Phase of Cesium Lead Iodide. *Nano Letters*, **2016**, 16, 3563-70	11.5	208
64	Optical phonons in methylammonium lead halide perovskites and implications for charge transport. *Materials Horizons*, **2016**, 3, 613-620	14.4	228
63	Perovskite Solar Cells: Do We Know What We Do Not Know?. *Journal of Physical Chemistry Letters*, **2015**, 6, 279-82	6.4	65
62	Population inversion and giant bandgap renormalization in atomically thin WS2 layers. *Nature Photonics*, **2015**, 9, 466-470	33.9	260
61	Probing Interlayer Interactions in Transition Metal Dichalcogenide Heterostructures by Optical Spectroscopy: MoS2/WS2 and MoSe2/WSe2. *Nano Letters*, **2015**, 15, 5033-8	11.5	214
60	Excitons in ultrathin organic-inorganic perovskite crystals. *Physical Review B*, **2015**, 92,	3.3	206
59	Reliable energy level alignment at physisorbed molecule-metal interfaces from density functional theory. *Nano Letters*, **2015**, 15, 2448-55	11.5	88
58	Electronic Properties of Biphenylthiolates on Au(111): The Impact of Coverage Revisited. *Journal of Physical Chemistry C*, **2015**, 119, 7817-7825	3.8	19
57	Observation of biexcitons in monolayer WSe2. *Nature Physics*, **2015**, 11, 477-481	16.2	399
56	Impact of Anchoring Groups on Ballistic Transport: Single Molecule vs Monolayer Junctions. *Journal of Physical Chemistry C*, **2015**, 119, 21198-21208	3.8	36
55	Are Mobilities in Hybrid Organic-Inorganic Halide Perovskites Actually "High"?. *Journal of Physical Chemistry Letters*, **2015**, 6, 4754-7	6.4	167
54	Bright and dark singlet excitons via linear and two-photon spectroscopy in monolayer transition-metal dichalcogenides. *Physical Review B*, **2015**, 92,	3.3	54
53	Binding energies and spatial structures of small carrier complexes in monolayer transition-metal dichalcogenides via diffusion Monte Carlo. *Physical Review B*, **2015**, 92,	3.3	64
52	Electrical Tuning of Exciton Binding Energies in Monolayer WS_{2}. *Physical Review Letters*, **2015**, 115, 126802	7.4	248
51	Microscopic Dynamics of Supercooled Liquids from First Principles. *Physical Review Letters*, **2015**, 115, 205701	7.4	46
50	Taming the Dynamical Sign Problem in Real-Time Evolution of Quantum Many-Body Problems. *Physical Review Letters*, **2015**, 115, 266802	7.4	86

49	Extending the applicability of Redfield theories into highly non-Markovian regimes. *Journal of Chemical Physics*, **2015**, 143, 194108	3.9	33
48	Hybrid Organic-Inorganic Perovskites (HOIPs): Opportunities and Challenges. *Advanced Materials*, **2015**, 27, 5102-12	24	325
47	The Effects of Embedded Dipoles in Aromatic Self-Assembled Monolayers. *Advanced Functional Materials*, **2015**, 25, 3943-3957	15.6	73
46	Theory of hydrogen migration in organic-inorganic halide perovskites. *Angewandte Chemie - International Edition*, **2015**, 54, 12437-41	16.4	112
45	Tuning the Electronic Structure of Graphene through Collective Electrostatic Effects. *Advanced Materials Interfaces*, **2015**, 2, 1500323	4.6	8
44	Absence of diffusion in an interacting system of spinless fermions on a one-dimensional disordered lattice. *Physical Review Letters*, **2015**, 114, 100601	7.4	197
43	A Toolbox for Controlling the Energetics and Localization of Electronic States in Self-Assembled Organic Monolayers. *Advanced Science*, **2015**, 2, 1400016	13.6	17
42	Green functions from real-time bold-line Monte Carlo calculations: spectral properties of the nonequilibrium Anderson impurity model. *Physical Review Letters*, **2014**, 112, 146802	7.4	64
41	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	6.4	109
40	Correlation of local order with particle mobility in supercooled liquids is highly system dependent. *Physical Review Letters*, **2014**, 113, 157801	7.4	69
39	Impact of Collective Electrostatic Effects on Charge Transport through Molecular Monolayers. *Journal of Physical Chemistry C*, **2014**, 118, 22395-22401	3.8	20
38	Spectroscopic Study of Anisotropic Excitons in Single Crystal Hexacene. *Journal of Physical Chemistry Letters*, **2014**, 5, 3632-5	6.4	7
37	Role of Dispersive Interactions in Determining Structural Properties of Organic-Inorganic Halide Perovskites: Insights from First-Principles Calculations. *Journal of Physical Chemistry Letters*, **2014**, 5, 2728-33	6.4	168
36	Exciton binding energy and nonhydrogenic Rydberg series in monolayer WS(2). *Physical Review Letters*, **2014**, 113, 076802	7.4	1358
35	Crossovers in the dynamics of supercooled liquids probed by an amorphous wall. *Physical Review E*, **2014**, 89, 052311	2.4	31
34	Green functions from real-time bold-line Monte Carlo. *Physical Review B*, **2014**, 89,	3.3	35
33	Understanding the adsorption of CuPc and ZnPc on noble metal surfaces by combining quantum-mechanical modelling and photoelectron spectroscopy. *Molecules*, **2014**, 19, 2969-92	4.8	66
32	Relaxation patterns in supercooled liquids from generalized mode-coupling theory. *Physical Review E*, **2014**, 90, 052306	2.4	23

31	Critical dynamical heterogeneities close to continuous second-order glass transitions. *Physical Review Letters*, **2014**, 113, 245701	7.4	11
30	Equilibrium ultrastable glasses produced by random pinning. *Journal of Chemical Physics*, **2014**, 141, 224503	3.3	26
29	Microscopic theory of singlet exciton fission. III. Crystalline pentacene. *Journal of Chemical Physics*, **2014**, 141, 074705	3.9	135
28	Measurement of the optical dielectric function of monolayer transition-metal dichalcogenides: MoS2, MoSe2, WS2, and WSe2. *Physical Review B*, **2014**, 90,	3.3	739
27	Valley splitting and polarization by the Zeeman effect in monolayer MoSe2. *Physical Review Letters*, **2014**, 113, 266804	7.4	299
26	Effect of Molecule-Surface Reaction Mechanism on the Electronic Characteristics and Photovoltaic Performance of Molecularly Modified Si. *Journal of Physical Chemistry C*, **2013**, 117, 22351-22361	3.8	21
25	Theory of neutral and charged excitons in monolayer transition metal dichalcogenides. *Physical Review B*, **2013**, 88,	3.3	579
24	Anticorrelation between the Evolution of Molecular Dipole Moments and Induced Work Function Modifications. *Journal of Physical Chemistry Letters*, **2013**, 4, 3521-3526	6.4	19
23	The quantum coherent mechanism for singlet fission: experiment and theory. *Accounts of Chemical Research*, **2013**, 46, 1321-9	24.3	214
22	Understanding Structure and Bonding of Multilayered Metal-Organic Nanostructures. *Journal of Physical Chemistry C*, **2013**, 117, 3055-3061	3.8	36
21	Numerically exact long-time magnetization dynamics at the nonequilibrium Kondo crossover of the Anderson impurity model. *Physical Review B*, **2013**, 87,	3.3	94
20	Accurate Force Field Development for Modeling Conjugated Polymers. *Journal of Chemical Theory and Computation*, **2012**, 8, 4556-69	6.4	85
19	Finite-temperature auxiliary-field quantum Monte Carlo technique for Bose-Fermi mixtures. *Physical Review A*, **2012**, 86,	2.6	23
18	Dimensionality effects in the electronic structure of organic semiconductors consisting of polar repeat units. *Organic Electronics*, **2012**, 13, 3165-3176	3.5	19
17	Polarity switching of charge transport and thermoelectricity in self-assembled monolayer devices. *Advanced Materials*, **2012**, 24, 4403-7	24	21
16	Collectively induced quantum-confined Stark effect in monolayers of molecules consisting of polar repeating units. *Journal of the American Chemical Society*, **2011**, 133, 18634-45	16.4	31
15	Quantum fluctuations can promote or inhibit glass formation. *Nature Physics*, **2011**, 7, 134-137	16.2	74
14	Quantum quench spectroscopy of a Luttinger liquid: Ultrarelativistic density wave dynamics due to fractionalization in an XXZ chain. *Physical Review B*, **2011**, 84,	3.3	19

13	Numerically exact long-time behavior of nonequilibrium quantum impurity models. *Physical Review B*, **2011**, 84,	3.3	41
12	Transport through a quantum dot with excitonic dot-lead coupling. *Physical Review B*, **2011**, 83,	3.3	7
11	Transport through a quantum dot with two parallel Luttinger liquid leads. *Physical Review B*, **2011**, 83,	3.3	8
10	Effect of a Coulombic dot-lead coupling on the dynamics of a quantum dot. *Physical Review B*, **2010**, 81,	3.3	14
9	Bold-line diagrammatic Monte Carlo method: General formulation and application to expansion around the noncrossing approximation. *Physical Review B*, **2010**, 82,	3.3	55
8	Work-function modification beyond pinning: when do molecular dipoles count?. *Nano Letters*, **2010**, 10, 4369-74	11.5	63
7	The electronic structure of mixed self-assembled monolayers. *ACS Nano*, **2010**, 4, 6735-46	16.7	34
6	Self-assembled monolayers of polar molecules on Au(111) surfaces: distributing the dipoles. *Physical Chemistry Chemical Physics*, **2010**, 12, 4291-4	3.6	24
5	Analytic continuation average spectrum method for quantum liquids. *Journal of Chemical Physics*, **2009**, 131, 054502	3.9	12
4	Irreversible reorganization in a supercooled liquid originates from localized soft modes. *Nature Physics*, **2008**, 4, 711-715	16.2	308
3	On the Role of Hydrodynamic Interactions in Colloidal Gelation. *Journal of the Physical Society of Japan*, **2008**, 77, 084804	1.5	24
2	On stochastic models of dynamic disorder. *Journal of Physical Chemistry B*, **2006**, 110, 19061-5	3.4	5
1	Comparison of dynamical heterogeneity in hard-sphere and attractive glass formers. *Journal of Physical Chemistry B*, **2005**, 109, 14654-8	3.4	48