David R Reichman

List of Publications by Year in Descending Order

126 papers	12,906 citations	49 h-index	113 g-index
135 ext. papers	14,518 ext. citations	8.2 avg, IF	6.64 L-index

#	Paper	IF	Citations
126	Unbiasing fermionic quantum Monte Carlo with a quantum computer.. *Nature*, **2022**, 603, 416-420	50.4	10
125	Strongly Correlated Ladders in K-Doped -Terphenyl Crystals. *Nano Letters*, **2021**, 21, 9573-9579	11.5	
124	Time evolution of ML-MCTDH wavefunctions. II. Application of the projector splitting integrator. *Journal of Chemical Physics*, **2021**, 155, 174109	3.9	1
123	Time evolution of ML-MCTDH wavefunctions. I. Gauge conditions, basis functions, and singularities. *Journal of Chemical Physics*, **2021**, 155, 174108	3.9	2
122	Superatomic solid solutions. *Nature Chemistry*, **2021**, 13, 607-613	17.6	4
121	Spectral Functions from Auxiliary-Field Quantum Monte Carlo without Analytic Continuation: The Extended KoopmansTTheorem Approach. *Journal of Chemical Theory and Computation*, **2021**, 17, 3372-3387	6.4	5
120	The Significance of Polarons and Dynamic Disorder in Halide Perovskites. *ACS Energy Letters*, **2021**, 6, 2162-2173	20.1	17
119	Stochastic resolution-of-the-identity auxiliary-field quantum Monte Carlo: Scaling reduction without overhead. *Journal of Chemical Physics*, **2020**, 153, 044131	3.9	8
118	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
117	Depletion of Two-Level Systems in Ultrastable Computer-Generated Glasses. *Physical Review Letters*, **2020**, 124, 225901	7.4	20
116	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
115	Microscopic model of the doping dependence of linewidths in monolayer transition metal dichalcogenides. *Journal of Chemical Physics*, **2020**, 152, 194705	3.9	8
114	Studying dynamics in two-dimensional quantum lattices using tree tensor network states. *SciPost Physics*, **2020**, 9,	6.1	6
113	Molecular Engineering of Chromophores to Enable Triplet-Triplet Annihilation Upconversion. *Journal of the American Chemical Society*, **2020**, 142, 19917-19925	16.4	13
112	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
111	Multiset Matrix Product State Calculations Reveal Mobile Franck-Condon Excitations Under Strong Holstein-Type Coupling. *Physical Review Letters*, **2019**, 123, 126601	7.4	21
110	On mean-field theories of dynamics in supercooled liquids. *Journal of Chemical Physics*, **2019**, 151, 084503	3.9	9

109	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
108	Many-body theory of optical absorption in doped two-dimensional semiconductors. *Physical Review B*, **2019**, 99,	3.3	14
107	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
106	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
105	Removing instabilities in the hierarchical equations of motion: Exact and approximate projection approaches. *Journal of Chemical Physics*, **2019**, 150, 184109	3.9	26
104	Interlayer Excitons in Transition-Metal Dichalcogenide Heterobilayers. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1900308	1.3	7
103	Time-dependent variational principle in matrix-product state manifolds: Pitfalls and potential. *Physical Review B*, **2018**, 97,	3.3	32
102	Optical and Excitonic Properties of Atomically Thin Transition-Metal Dichalcogenides. *Annual Review of Condensed Matter Physics*, **2018**, 9, 379-396	19.7	46
101	Generalization of fewest-switches surface hopping for coherences. *Journal of Chemical Physics*, **2018**, 148, 102309	3.9	10
100	Momentum-space indirect interlayer excitons in transition-metal dichalcogenide van der Waals heterostructures. *Nature Physics*, **2018**, 14, 801-805	16.2	145
99	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
98	Phaseless Auxiliary-Field Quantum Monte Carlo on Graphical Processing Units. *Journal of Chemical Theory and Computation*, **2018**, 14, 4109-4121	6.4	25
97	How Lattice and Charge Fluctuations Control Carrier Dynamics in Halide Perovskites. *Nano Letters*, **2018**, 18, 8041-8046	11.5	51
96	Transient superconductivity from electronic squeezing of optically pumped phonons. *Nature Physics*, **2017**, 13, 479-483	16.2	104
95	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
94	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
93	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
92	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

91	Single-crystal-to-single-crystal intercalation of a low-bandgap superatomic crystal. *Nature Chemistry* , **2017**, 9, 1170-1174	17.6	44
90	Transport in quasiperiodic interacting systems: From superdiffusion to subdiffusion. *Europhysics Letters*, **2017**, 119, 37003	1.6	46
89	Atomistic Interrogation of B-N Co-dopant Structures and Their Electronic Effects in Graphene. *ACS Nano*, **2016**, 10, 6574-84	16.7	42
88	Energy Transfer from Quantum Dots to Graphene and MoS2: The Role of Absorption and Screening in Two-Dimensional Materials. *Nano Letters*, **2016**, 16, 2328-33	11.5	140
87	Slow dynamics in a two-dimensional Anderson-Hubbard model. *Europhysics Letters*, **2016**, 113, 46001	1.6	45
86	On the accuracy of surface hopping dynamics in condensed phase non-adiabatic problems. *Journal of Chemical Physics*, **2016**, 144, 094104	3.9	35
85	On the accuracy of the Padé-resummed master equation approach to dissipative quantum dynamics. *Journal of Chemical Physics*, **2016**, 144, 154106	3.9	15
84	Approximate but accurate quantum dynamics from the Mori formalism: I. Nonequilibrium dynamics. *Journal of Chemical Physics*, **2016**, 144, 184104	3.9	40
83	Observation of biexcitons in monolayer WSe2. *Nature Physics*, **2015**, 11, 477-481	16.2	399
82	Observation of Excitonic Rydberg States in Monolayer MoS2 and WS2 by Photoluminescence Excitation Spectroscopy. *Nano Letters*, **2015**, 15, 2992-7	11.5	259
81	Algorithm independent bounds on community detection problems and associated transitions in stochastic block model graphs. *Journal of Complex Networks*, **2015**, 3, 333-360	1.7	4
80	Microscopic Dynamics of Supercooled Liquids from First Principles. *Physical Review Letters*, **2015**, 115, 205701	7.4	46
79	Taming the Dynamical Sign Problem in Real-Time Evolution of Quantum Many-Body Problems. *Physical Review Letters*, **2015**, 115, 266802	7.4	86
78	Extending the applicability of Redfield theories into highly non-Markovian regimes. *Journal of Chemical Physics*, **2015**, 143, 194108	3.9	33
77	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
76	Green's 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
75	Segregation of sublattice domains in nitrogen-doped graphene. *Journal of the American Chemical Society*, **2014**, 136, 1391-7	16.4	73
74	Correlation of local order with particle mobility in supercooled liquids is highly system dependent. *Physical Review Letters*, **2014**, 113, 157801	7.4	69

73	Multiphonon relaxation slows singlet fission in crystalline hexacene. *Journal of the American Chemical Society*, **2014**, 136, 10654-60	16.4	92
72	Length-dependent conductance of oligothiophenes. *Journal of the American Chemical Society*, **2014**, 136, 10486-92	16.4	107
71	Exciton binding energy and nonhydrogenic Rydberg series in monolayer WS(2). *Physical Review Letters*, **2014**, 113, 076802	7.4	1358
70	Tailoring the electronic structure in bilayer molybdenum disulfide via interlayer twist. *Nano Letters*, **2014**, 14, 3869-75	11.5	213
69	Critical dynamical heterogeneities close to continuous second-order glass transitions. *Physical Review Letters*, **2014**, 113, 245701	7.4	11
68	Equilibrium ultrastable glasses produced by random pinning. *Journal of Chemical Physics*, **2014**, 141, 224503	3.9	26
67	Impact of molecular symmetry on single-molecule conductance. *Journal of the American Chemical Society*, **2013**, 135, 11724-7	16.4	49
66	Chromophore-Controlled Self-Assembly of Highly Ordered Polymer Nanostructures. *Journal of Physical Chemistry Letters*, **2013**, 4, 2520-2524	6.4	21
65	Theory of neutral and charged excitons in monolayer transition metal dichalcogenides. *Physical Review B*, **2013**, 88,	3.3	579
64	Local atomic and electronic structure of boron chemical doping in monolayer graphene. *Nano Letters*, **2013**, 13, 4659-65	11.5	168
63	Coherent quantum dynamics in donor□bridge□cceptor systems: beyond the hopping and super-exchange mechanisms. *New Journal of Physics*, **2013**, 15, 105020	2.9	26
62	Microscopic theory of singlet exciton fission. II. Application to pentacene dimers and the role of superexchange. *Journal of Chemical Physics*, **2013**, 138, 114103	3.9	260
61	The promoter-search mechanism of Escherichia coli RNA polymerase is dominated by three-dimensional diffusion. *Nature Structural and Molecular Biology*, **2013**, 20, 174-81	17.6	88
60	Dynamic length scales in glass-forming liquids: an inhomogeneous molecular dynamics simulation approach. *Journal of Physical Chemistry B*, **2013**, 117, 13259-67	3.4	6
59	The quantum coherent mechanism for singlet fission: experiment and theory. *Accounts of Chemical Research*, **2013**, 46, 1321-9	24.3	214
58	Microscopic theory of singlet exciton fission. I. General formulation. *Journal of Chemical Physics*, **2013**, 138, 114102	3.9	182
57	Grains and grain boundaries in highly crystalline monolayer molybdenum disulphide. *Nature Materials*, **2013**, 12, 554-61	27	1590
56	A small subset of normal modes mimics the properties of dynamical heterogeneity in a model supercooled liquid. *Journal of Chemical Physics*, **2013**, 138, 12A537	3.9	12

55	Accurate Force Field Development for Modeling Conjugated Polymers. *Journal of Chemical Theory and Computation*, **2012**, 8, 4556-69	6.4	85
54	Connecting dopant bond type with electronic structure in N-doped graphene. *Nano Letters*, **2012**, 12, 4025-31	11.5	381
53	Growing point-to-set length scale correlates with growing relaxation times in model supercooled liquids. *Physical Review Letters*, **2012**, 108, 225506	7.4	115
52	Visualizing individual nitrogen dopants in monolayer graphene. *Science*, **2011**, 333, 999-1003	33.3	697
51	Quantum fluctuations can promote or inhibit glass formation. *Nature Physics*, **2011**, 7, 134-137	16.2	74
50	Controlling chain conformation in conjugated polymers using defect inclusion strategies. *Journal of the American Chemical Society*, **2011**, 133, 10155-60	16.4	47
49	Nonequilibrium transport in quantum impurity models: exact path integral simulations. *Physical Chemistry Chemical Physics*, **2011**, 13, 14378-86	3.6	23
48	Analytic continuation average spectrum method for transport in quantum liquids. *Chemical Physics*, **2010**, 370, 132-136	2.3	6
47	Spatial dimension and the dynamics of supercooled liquids. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 15171-5	11.5	58
46	Localized soft modes and the supercooled liquid's irreversible passage through its configuration space. *Journal of Chemical Physics*, **2009**, 131, 194508	3.9	78
45	Soft colloids make strong glasses. *Nature*, **2009**, 462, 83-6	50.4	417
44	Irreversible reorganization in a supercooled liquid originates from localized soft modes. *Nature Physics*, **2008**, 4, 711-715	16.2	308
43	The subdiffusive targeting problem. *Journal of Physical Chemistry B*, **2008**, 112, 4283-9	3.4	15
42	Numerical investigation of glassy dynamics in low-density systems. *Physical Review Letters*, **2008**, 100, 195701	7.4	26
41	Strain-rate frequency superposition: a rheological probe of structural relaxation in soft materials. *Physical Review Letters*, **2007**, 98, 238303	7.4	195
40	Dynamic basis for one-dimensional DNA scanning by the mismatch repair complex Msh2-Msh6. *Molecular Cell*, **2007**, 28, 359-70	17.6	186
39	Cooperativity beyond caging: Generalized mode-coupling theory. *Physical Review Letters*, **2006**, 97, 095702	7.4	64
38	Contribution of slow clusters to the bulk elasticity near the colloidal glass transition. *Physical Review Letters*, **2006**, 97, 265701	7.4	42

37	Inhomogeneous mode-coupling theory and growing dynamic length in supercooled liquids. *Physical Review Letters*, **2006**, 97, 195701	7.4	241
36	On stochastic models of dynamic disorder. *Journal of Physical Chemistry B*, **2006**, 110, 19061-5	3.4	5
35	Tribute to Robert J. Silbey. *Journal of Physical Chemistry B*, **2006**, 110, 18734-18734	3.4	
34	Comparison of dynamical heterogeneity in hard-sphere and attractive glass formers. *Journal of Physical Chemistry B*, **2005**, 109, 14654-8	3.4	48
33	Effect of flexibility on hydrophobic behavior of nanotube water channels. *Journal of Chemical Physics*, **2005**, 123, 194502	3.9	69
32	Quantum mode-coupling theory: formulation and applications to normal and supercooled quantum liquids. *Annual Review of Physical Chemistry*, **2005**, 56, 157-85	15.7	30
31	Magnetic self-assembly of three-dimensional surfaces from planar sheets. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 3924-9	11.5	112
30	Transport properties of normal liquid helium: comparison of various methodologies. *Journal of Chemical Physics*, **2005**, 123, 184506	3.9	18
29	Mode-coupling theory. *Journal of Statistical Mechanics: Theory and Experiment*, **2005**, 2005, P05013	1.9	187
28	Semiclassical representations of electronic structure and dynamics. *Journal of Chemical Physics*, **2004**, 120, 579-89	3.9	10
27	A fully self-consistent treatment of collective fluctuations in quantum liquids. *Journal of Chemical Physics*, **2004**, 120, 1458-65	3.9	47
26	Critical tests of a new master equation approach to nonadiabatic quantum dissipative systems. *Chemical Physics*, **2004**, 296, 129-134	2.3	11
25	Relationship between Mechanical and Dynamical Properties of Glass Forming Liquids *Journal of Physical Chemistry B*, **2004**, 108, 19703-19710	3.4	10
24	Numerical Investigation of the Entropy Crisis in Model Glass Formers *Journal of Physical Chemistry B*, **2004**, 108, 6832-6837	3.4	23
23	Drying-mediated self-assembly of nanoparticles. *Nature*, **2003**, 426, 271-4	50.4	806
22	Analytic continuation for quantum nonadiabatic rate constants. *Journal of Chemical Physics*, **2003**, 118, 457-460	3.9	27
21	Molecular hydrodynamic theory of nonresonant Raman spectra in liquids: Third-order spectra. *Journal of Chemical Physics*, **2002**, 116, 1979-1986	3.9	15
20	A self-consistent mode-coupling theory for dynamical correlations in quantum liquids: Application to liquid para-hydrogen. *Journal of Chemical Physics*, **2002**, 116, 6279-6285	3.9	60

19	Molecular hydrodynamic theory of nonresonant Raman spectra in liquids: Fifth-order spectra. *Journal of Chemical Physics*, **2002**, 116, 1987-1994	3.9	23
18	Adaptive nudged elastic band approach for transition state calculation. *Journal of Chemical Physics*, **2002**, 117, 4651-4658	3.9	138
17	A self-consistent mode-coupling theory for dynamical correlations in quantum liquids: Rigorous formulation. *Journal of Chemical Physics*, **2002**, 116, 6271-6278	3.9	50
16	Calculating approximate quantum mechanical rates without an a priori reaction coordinate. *Journal of Chemical Physics*, **2002**, 116, 8376	3.9	6
15	The calculation of transport properties in quantum liquids using the maximum entropy numerical analytic continuation method: application to liquid para-hydrogen. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 1129-33	11.5	88
14	On the multiple time scales in solvation dynamics: A mode-coupling theory approach. *Journal of Chemical Physics*, **2002**, 116, 5080	3.9	24
13	Classical mapping approaches for nonadiabatic dynamics: Short time analysis. *Journal of Chemical Physics*, **2001**, 114, 1065-1074	3.9	42
12	Reference system master equation approaches to condensed phase charge transfer processes. II. Numerical tests and applications to the study of photoinduced charge transfer reactions. *Journal of Chemical Physics*, **2001**, 115, 9862-9870	3.9	28
11	Self-consistent mode-coupling theory for self-diffusion in quantum liquids. *Physical Review Letters*, **2001**, 87, 265702	7.4	58
10	Reference system master equation approaches to condensed phase charge transfer processes. I. General formulation. *Journal of Chemical Physics*, **2001**, 115, 9848-9861	3.9	37
9	A Short-Time Quantum Mechanical Expansion Approach to Vibrational Relaxation *Journal of Physical Chemistry B*, **2001**, 105, 6550-6555	3.4	26
8	A Feynman path centroid dynamics approach for the computation of time correlation functions involving nonlinear operators. *Journal of Chemical Physics*, **2000**, 113, 919-929	3.9	88
7	Self-consistent harmonic theory of solvation in glassy systems: Quantum solvation. *Journal of Chemical Physics*, **2000**, 112, 3280-3284	3.9	3
6	Self-consistent harmonic theory of solvation in glassy systems: Classical solvation. *Journal of Chemical Physics*, **2000**, 112, 3267-3279	3.9	2
5	Spectral diffusion on ultralong time scales in low-temperature glasses. *Physical Review B*, **1997**, 56, 5250-5260	3.7	21
4	Cumulant expansions and the spin-boson problem. *Physical Review E*, **1997**, 55, 2328-2337	2.4	29
3	On the relaxation of a two-level system: Beyond the weak-coupling approximation. *Journal of Chemical Physics*, **1996**, 104, 1506-1518	3.9	47
2	On the nonperturbative theory of pure dephasing in condensed phases at low temperatures. *Journal of Chemical Physics*, **1996**, 105, 10500-10506	3.9	25

1	Alternative model of dissipation in quantum mechanics. *Physical Review E*, **1996**, 53, 4184-4186	2.4	2