David R Reichman

List of Publications by Year
in descending order

134 papers	15,901 citations	30070 54 h-index	15732 125 g-index
135 all docs	135 docs citations	135 times ranked	18741 citing authors

#	Article	IF	Citations
1	Unbiasing fermionic quantum Monte Carlo with a quantum computer. Nature, 2022, 603, 416-420.	27.8	84
2	A Localized-Orbital Energy Evaluation for Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2022, 18, 3447-3459.	5.3	7
3	Cumulant methods for electron-phonon problems. I. Perturbative expansions. Physical Review B, 2022, 105, .	3.2	5
4	2D materials. Journal of Chemical Physics, 2021, 154, 040401.	3.0	1
5	Superatomic solid solutions. Nature Chemistry, 2021, 13, 607-613.	13.6	15
6	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.	5.3	10
7	The Significance of Polarons and Dynamic Disorder in Halide Perovskites. ACS Energy Letters, 2021, 6, 2162-2173.	17.4	74
8	Time evolution of ML-MCTDH wavefunctions. II. Application of the projector splitting integrator. Journal of Chemical Physics, 2021, 155, 174109.	3.0	5
9	Time evolution of ML-MCTDH wavefunctions. I. Gauge conditions, basis functions, and singularities. Journal of Chemical Physics, 2021, 155, 174108.	3.0	7
10	Strongly Correlated Ladders in K-Doped p-Terphenyl Crystals. Nano Letters, 2021, 21, 9573-9579.	9.1	1
11	2020 JCP Emerging Investigator Special Collection. Journal of Chemical Physics, 2021, 155, 230401.	3.0	1
12	JCP Emerging Investigator Special Collection 2019. Journal of Chemical Physics, 2020, 153, 110402.	3.0	2
13	Molecular Engineering of Chromophores to Enable Tripletâ€“Triplet Annihilation Upconversion. Journal of the American Chemical Society, 2020, 142, 19917-19925.	13.7	42
14	Singlet fission. Journal of Chemical Physics, 2020, 153, 110401.	3.0	3
15	Chemical physics of materials. Journal of Chemical Physics, 2020, 153, 100402.	3.0	0
16	Stochastic resolution-of-the-identity auxiliary-field quantum Monte Carlo: Scaling reduction without overhead. Journal of Chemical Physics, 2020, 153, 044131.	3.0	15
17	The performance of phaseless auxiliary-field quantum Monte Carlo on the ground state electronic energy of benzene. Journal of Chemical Physics, 2020, 153, 126101.	3.0	17
18	Depletion of Two-Level Systems in Ultrastable Computer-Generated Glasses. Physical Review Letters, 2020, 124, 225901.	7.8	47

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19	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.	13.7	9
20	Microscopic model of the doping dependence of linewidths in monolayer transition metal dichalcogenides. Journal of Chemical Physics, 2020, 152, 194705.	3.0	15
21	Predicting Ligand-Dissociation Energies of 3d Coordination Complexes with Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2020, 16, 3041-3054.	5.3	21
22	Studying dynamics in two-dimensional quantum lattices using tree tensor network states. SciPost Physics, 2020, 9, .	4.9	13
23	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.	5.3	37
24	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.	3.1	91
25	Removing instabilities in the hierarchical equations of motion: Exact and approximate projection approaches. Journal of Chemical Physics, 2019, 150, 184109.	3.0	46
26	Interlayer Excitons in Transitionâ€Metal Dichalcogenide Heterobilayers. Physica Status Solidi (B): Basic Research, 2019, 256, 1900308.	1.5	15
27	Multiset Matrix Product State Calculations Reveal Mobile Franck-Condon Excitations Under Strong Holstein-Type Coupling. Physical Review Letters, 2019, 123, 126601.	7.8	35
28	On mean-field theories of dynamics in supercooled liquids. Journal of Chemical Physics, 2019, 151, 084503.	3.0	13
29	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.	5.3	62
30	Many-body theory of optical absorption in doped two-dimensional semiconductors. Physical Review B, 2019, 99, .	3.2	28
31	Time-dependent variational principle in matrix-product state manifolds: Pitfalls and potential. Physical Review B, 2018, 97, .	3.2	49
32	Optical and Excitonic Properties of Atomically Thin Transition-Metal Dichalcogenides. Annual Review of Condensed Matter Physics, 2018, 9, 379-396.	14.5	68
33	Generalization of fewest-switches surface hopping for coherences. Journal of Chemical Physics, 2018, 148, 102309.	3.0	15
34	Momentum-space indirect interlayer excitons in transition-metal dichalcogenide van der Waals heterostructures. Nature Physics, 2018, 14, 801-805.	16.7	229
35	How Lattice and Charge Fluctuations Control Carrier Dynamics in Halide Perovskites. Nano Letters, 2018, 18, 8041-8046.	9.1	97
36	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.	3.0	67

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37	Phaseless Auxiliary-Field Quantum Monte Carlo on Graphical Processing Units. Journal of Chemical Theory and Computation, 2018, 14, 4109-4121.	5.3	35
38	Transient superconductivity from electronic squeezing of optically pumped phonons. Nature Physics, 2017, 13, 479-483.	16.7	139
39	Vibronic exciton theory of singlet fission. II. Two-dimensional spectroscopic detection of the correlated triplet pair state. Journal of Chemical Physics, 2017, 146, 174704.	3.0	53
40	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.	3.0	77
41	Chemical Transformations Approaching Chemical Accuracy via Correlated Sampling in Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2017, 13, 2667-2680.	5.3	33
42	Triplet Separation Drives Singlet Fission after Femtosecond Correlated Triplet Pair Production in Rubrene. Journal of the American Chemical Society, 2017, 139, 11745-11751.	13.7	107
43	Single-crystal-to-single-crystal intercalation of a low-bandgap superatomic crystal. Nature Chemistry, 2017, 9, 1170-1174.	13.6	56
44	Transport in quasiperiodic interacting systems: From superdiffusion to subdiffusion. Europhysics Letters, 2017, 119, 37003.	2.0	70
45	Slow dynamics in a two-dimensional Anderson-Hubbard model. Europhysics Letters, 2016, 113, 46001.	2.0	52
46	On the accuracy of surface hopping dynamics in condensed phase non-adiabatic problems. Journal of Chemical Physics, 2016, 144, 094104.	3.0	43
47	On the accuracy of the PadÃ©-resummed master equation approach to dissipative quantum dynamics. Journal of Chemical Physics, 2016, 144, 154106.	3.0	17
48	Approximate but accurate quantum dynamics from the Mori formalism: I. Nonequilibrium dynamics. Journal of Chemical Physics, 2016, 144, 184104.	3.0	48
49	Atomistic Interrogation of Bâ€“N Co-dopant Structures and Their Electronic Effects in Graphene. ACS Nano, 2016, 10, 6574-6584.	14.6	53
50	Energy Transfer from Quantum Dots to Graphene and MoS₂: The Role of Absorption and Screening in Two-Dimensional Materials. Nano Letters, 2016, 16, 2328-2333.	9.1	179
51	Algorithm independent bounds on community detection problems and associated transitions in stochastic block model graphs. Journal of Complex Networks, 2015, 3, 333-360.	1.8	5
52	Microscopic Dynamics of Supercooled Liquids from First Principles. Physical Review Letters, 2015, 115, 205701.	7.8	62
53	Taming the Dynamical Sign Problem in Real-Time Evolution of Quantum Many-Body Problems. Physical Review Letters, 2015, 115, 266802.	7.8	138
54	Extending the applicability of Redfield theories into highly non-Markovian regimes. Journal of Chemical Physics, 2015, 143, 194108.	3.0	41

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55	Absence of Diffusion in an Interacting System of Spinless Fermions on a One-Dimensional Disordered Lattice. Physical Review Letters, 2015, 114, 100601.	7.8	246
56	Observation of biexcitons in monolayer WSe2. Nature Physics, 2015, 11, 477-481.	16.7	531
57	Observation of Excitonic Rydberg States in Monolayer MoS₂ and WS₂ by Photoluminescence Excitation Spectroscopy. Nano Letters, 2015, 15, 2992-2997.	9.1	327
58	Critical Dynamical Heterogeneities Close to Continuous Second-Order Glass Transitions. Physical Review Letters, 2014, 113, 245701.	7.8	13
59	Equilibrium ultrastable glasses produced by random pinning. Journal of Chemical Physics, 2014, 141, 224503.	3.0	31
60	Greenâ€™s Functions from Real-Time Bold-Line MonteÂCarlo Calculations: Spectral Properties of the Nonequilibrium Anderson Impurity Model. Physical Review Letters, 2014, 112, 146802.	7.8	80
61	Segregation of Sublattice Domains in Nitrogen-Doped Graphene. Journal of the American Chemical Society, 2014, 136, 1391-1397.	13.7	86
62	Correlation of Local Order with Particle Mobility in Supercooled Liquids Is Highly System Dependent. Physical Review Letters, 2014, 113, 157801.	7.8	83
63	Multiphonon Relaxation Slows Singlet Fission in Crystalline Hexacene. Journal of the American Chemical Society, 2014, 136, 10654-10660.	13.7	114
64	Length-Dependent Conductance of Oligothiophenes. Journal of the American Chemical Society, 2014, 136, 10486-10492.	13.7	127
65	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> Physical Review Letters, 2014, 113, 076802.	7.8	1,814
66	Tailoring the Electronic Structure in Bilayer Molybdenum Disulfide via Interlayer Twist. Nano Letters, 2014, 14, 3869-3875.	9.1	278
67	Impact of Molecular Symmetry on Single-Molecule Conductance. Journal of the American Chemical Society, 2013, 135, 11724-11727.	13.7	57
68	Chromophore-Controlled Self-Assembly of Highly Ordered Polymer Nanostructures. Journal of Physical Chemistry Letters, 2013, 4, 2520-2524.	4.6	22
69	Theory of neutral and charged excitons in monolayer transition metal dichalcogenides. Physical Review B, 2013, 88, .	3.2	737
70	Local Atomic and Electronic Structure of Boron Chemical Doping in Monolayer Graphene. Nano Letters, 2013, 13, 4659-4665.	9.1	192
71	Coherent quantum dynamics in donorâ€“bridgeâ€“acceptor systems: beyond the hopping and super-exchange mechanisms. New Journal of Physics, 2013, 15, 105020.	2.9	30
72	Microscopic theory of singlet exciton fission. II. Application to pentacene dimers and the role of superexchange. Journal of Chemical Physics, 2013, 138, 114103.	3.0	311

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73	The promoter-search mechanism of Escherichia coli RNA polymerase is dominated by three-dimensional diffusion. Nature Structural and Molecular Biology, 2013, 20, 174-181.	8.2	110
74	Dynamic Length Scales in Glass-Forming Liquids: An Inhomogeneous Molecular Dynamics Simulation Approach. Journal of Physical Chemistry B, 2013, 117, 13259-13267.	2.6	7
75	E. Coli RNA Polymerase Searches for Promoters through 3D Diffusion. Biophysical Journal, 2013, 104, 541a.	0.5	0
76	The Quantum Coherent Mechanism for Singlet Fission: Experiment and Theory. Accounts of Chemical Research, 2013, 46, 1321-1329.	15.6	262
77	Microscopic theory of singlet exciton fission. I. General formulation. Journal of Chemical Physics, 2013, 138, 114102.	3.0	210
78	Grains and grain boundaries in highly crystalline monolayer molybdenum disulphide. Nature Materials, 2013, 12, 554-561.	27.5	1,896
79	A small subset of normal modes mimics the properties of dynamical heterogeneity in a model supercooled liquid. Journal of Chemical Physics, 2013, 138, 12A537.	3.0	13
80	Accurate Force Field Development for Modeling Conjugated Polymers. Journal of Chemical Theory and Computation, 2012, 8, 4556-4569.	5.3	109
81	Connecting Dopant Bond Type with Electronic Structure in N-Doped Graphene. Nano Letters, 2012, 12, 4025-4031.	9.1	471
82	Growing Point-to-Set Length Scale Correlates with Growing Relaxation Times in Model Supercooled Liquids. Physical Review Letters, 2012, 108, 225506.	7.8	126
83	Nonequilibrium transport in quantum impurity models: exact path integral simulations. Physical Chemistry Chemical Physics, 2011, 13, 14378.	2.8	24
84	Visualizing Individual Nitrogen Dopants in Monolayer Graphene. Science, 2011, 333, 999-1003.	12.6	774
85	Quantum fluctuations can promote or inhibit glassÂformation. Nature Physics, 2011, 7, 134-137.	16.7	84
86	Controlling Chain Conformation in Conjugated Polymers Using Defect Inclusion Strategies. Journal of the American Chemical Society, 2011, 133, 10155-10160.	13.7	52
87	Analytic continuation average spectrum method for transport in quantum liquids. Chemical Physics, 2010, 370, 132-136.	1.9	6
88	Spatial dimension and the dynamics of supercooled liquids. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15171-15175.	7.1	68
89	Localized soft modes and the supercooled liquidâ€™s irreversible passage through its configuration space. Journal of Chemical Physics, 2009, 131, 194508.	3.0	83
90	Soft colloids make strong glasses. Nature, 2009, 462, 83-86.	27.8	464

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91	Irreversible reorganization in a supercooled liquid originates from localized soft modes. Nature Physics, 2008, 4, 711-715.	16.7	367
92	The Subdiffusive Targeting Problem. Journal of Physical Chemistry B, 2008, 112, 4283-4289.	2.6	16
93	Numerical Investigation of Glassy Dynamics in Low-Density Systems. Physical Review Letters, 2008, 100, 195701.	7.8	27
94	Dynamic Basis for One-Dimensional DNA Scanning by the Mismatch Repair Complex Msh2-Msh6. Molecular Cell, 2007, 28, 359-370.	9.7	215
95	Strain-Rate Frequency Superposition: A Rheological Probe of Structural Relaxation in Soft Materials. Physical Review Letters, 2007, 98, 238303.	7.8	220
96	Inhomogeneous Mode-Coupling Theory and Growing Dynamic Length in Supercooled Liquids. Physical Review Letters, 2006, 97, 195701.	7.8	262
97	On Stochastic Models of Dynamic Disorderâ€. Journal of Physical Chemistry B, 2006, 110, 19061-19065.	2.6	5
98	Tribute to Robert J. Silbey. Journal of Physical Chemistry B, 2006, 110, 18734-18734.	2.6	0
99	Cooperativity beyond Caging: Generalized Mode-Coupling Theory. Physical Review Letters, 2006, 97, 095702.	7.8	72
100	Contribution of Slow Clusters to the Bulk Elasticity Near the Colloidal Glass Transition. Physical Review Letters, 2006, 97, 265701.	7.8	45
101	QUANTUM MODE-COUPLING THEORY: Formulation and Applications to Normal and Supercooled Quantum Liquids. Annual Review of Physical Chemistry, 2005, 56, 157-185.	10.8	33
102	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, 3924-3929.	7.1	131
103	Transport properties of normal liquid helium: Comparison of various methodologies. Journal of Chemical Physics, 2005, 123, 184506.	3.0	18
104	Mode-coupling theory. Journal of Statistical Mechanics: Theory and Experiment, 2005, 2005, P05013.	2.3	228
105	Comparison of Dynamical Heterogeneity in Hard-Sphere and Attractive Glass Formersâ€. Journal of Physical Chemistry B, 2005, 109, 14654-14658.	2.6	49
106	Effect of flexibility on hydrophobic behavior of nanotube water channels. Journal of Chemical Physics, 2005, 123, 194502.	3.0	71
107	Semiclassical representations of electronic structure and dynamics. Journal of Chemical Physics, 2004, 120, 579-589.	3.0	10
108	A fully self-consistent treatment of collective fluctuations in quantum liquids. Journal of Chemical Physics, 2004, 120, 1458-1465.	3.0	47

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109	Critical tests of a new master equation approach to nonadiabatic quantum dissipative systems. Chemical Physics, 2004, 296, 129-134.	1.9	13
110	Relationship between Mechanical and Dynamical Properties of Glass Forming Liquidsâ€. Journal of Physical Chemistry B, 2004, 108, 19703-19710.	2.6	10
111	Numerical Investigation of the Entropy Crisis in Model Glass Formers. Journal of Physical Chemistry B, 2004, 108, 6832-6837.	2.6	28
112	Drying-mediated self-assembly of nanoparticles. Nature, 2003, 426, 271-274.	27.8	866
113	Analytic continuation for quantum nonadiabatic rate constants. Journal of Chemical Physics, 2003, 118, 457-460.	3.0	27
114	Molecular hydrodynamic theory of nonresonant Raman spectra in liquids: Third-order spectra. Journal of Chemical Physics, 2002, 116, 1979-1986.	3.0	16
115	A self-consistent mode-coupling theory for dynamical correlations in quantum liquids: Application to liquidpara-hydrogen. Journal of Chemical Physics, 2002, 116, 6279-6285.	3.0	60
116	Molecular hydrodynamic theory of nonresonant Raman spectra in liquids: Fifth-order spectra. Journal of Chemical Physics, 2002, 116, 1987-1994.	3.0	24
117	Adaptive nudged elastic band approach for transition state calculation. Journal of Chemical Physics, 2002, 117, 4651-4658.	3.0	148
118	A self-consistent mode-coupling theory for dynamical correlations in quantum liquids: Rigorous formulation. Journal of Chemical Physics, 2002, 116, 6271-6278.	3.0	52
119	Calculating approximate quantum mechanical rates without an a priori reaction coordinate. Journal of Chemical Physics, 2002, 116, 8376.	3.0	6
120	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, 1129-1133.	7.1	89
121	On the multiple time scales in solvation dynamics: A mode-coupling theory approach. Journal of Chemical Physics, 2002, 116, 5080.	3.0	24
122	Self-Consistent Mode-Coupling Theory for Self-Diffusion in Quantum Liquids. Physical Review Letters, 2001, 87, 265702.	7.8	61
123	Reference system master equation approaches to condensed phase charge transfer processes. I. General formulation. Journal of Chemical Physics, 2001, 115, 9848-9861.	3.0	39
124	A Short-Time Quantum Mechanical Expansion Approach to Vibrational Relaxationâ€. Journal of Physical Chemistry B, 2001, 105, 6550-6555.	2.6	26
125	Classical mapping approaches for nonadiabatic dynamics: Short time analysis. Journal of Chemical Physics, 2001, 114, 1065-1074.	3.0	45
126	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.	3.0	29

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127	A Feynman path centroid dynamics approach for the computation of time correlation functions involving nonlinear operators. Journal of Chemical Physics, 2000, 113, 919-929.	3.0	91
128	Self-consistent harmonic theory of solvation in glassy systems: Quantum solvation. Journal of Chemical Physics, 2000, 112, 3280-3284.	3.0	3
129	Self-consistent harmonic theory of solvation in glassy systems: Classical solvation. Journal of Chemical Physics, 2000, 112, 3267-3279.	3.0	4
130	Spectral diffusion on ultralong time scales in low-temperature glasses. Physical Review B, 1997, 56, 5250-5260.	3.2	21
131	Cumulant expansions and the spin-boson problem. Physical Review E, 1997, 55, 2328-2337.	2.1	30
132	On the relaxation of a twoâ€level system: Beyond the weakâ€coupling approximation. Journal of Chemical Physics, 1996, 104, 1506-1518.	3.0	49
133	On the nonperturbative theory of pure dephasing in condensed phases at low temperatures. Journal of Chemical Physics, 1996, 105, 10500-10506.	3.0	28
134	Alternative model of dissipation in quantum mechanics. Physical Review E, 1996, 53, 4184-4186.	2.1	2