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	Grains and grain boundaries in highly crystalline monolayer molybdenum disulphide. Nature Materials, 2013, 12, 554-561.	27.5	1,896
2	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></m Physical Review Letters, 2014, 113, 076802.	7.8	1,814
3	Drying-mediated self-assembly of nanoparticles. Nature, 2003, 426, 271-274.	27.8	866
4	Visualizing Individual Nitrogen Dopants in Monolayer Graphene. Science, 2011, 333, 999-1003.	12.6	774
5	Theory of neutral and charged excitons in monolayer transition metal dichalcogenides. Physical Review B, 2013, 88, .	3.2	737
6	Observation of biexcitons in monolayer WSe2. Nature Physics, 2015, 11, 477-481.	16.7	531
7	Connecting Dopant Bond Type with Electronic Structure in N-Doped Graphene. Nano Letters, 2012, 12, 4025-4031.	9.1	471
8	Soft colloids make strong glasses. Nature, 2009, 462, 83-86.	27.8	464
9	Irreversible reorganization in a supercooled liquid originates from localized soft modes. Nature Physics, 2008, 4, 711-715.	16.7	367
10	Observation of Excitonic Rydberg States in Monolayer MoS₂ and WS₂ by Photoluminescence Excitation Spectroscopy. Nano Letters, 2015, 15, 2992-2997.	9.1	327
11	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
12	Tailoring the Electronic Structure in Bilayer Molybdenum Disulfide via Interlayer Twist. Nano Letters, 2014, 14, 3869-3875.	9.1	278
13	Inhomogeneous Mode-Coupling Theory and Growing Dynamic Length in Supercooled Liquids. Physical Review Letters, 2006, 97, 195701.	7.8	262
14	The Quantum Coherent Mechanism for Singlet Fission: Experiment and Theory. Accounts of Chemical Research, 2013, 46, 1321-1329.	15.6	262
15	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
16	Momentum-space indirect interlayer excitons in transition-metal dichalcogenide van der Waals heterostructures. Nature Physics, 2018, 14, 801-805.	16.7	229
17	Mode-coupling theory. Journal of Statistical Mechanics: Theory and Experiment, 2005, 2005, P05013.	2.3	228
18	Strain-Rate Frequency Superposition: A Rheological Probe of Structural Relaxation in Soft Materials. Physical Review Letters, 2007, 98, 238303.	7.8	220

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19	Dynamic Basis for One-Dimensional DNA Scanning by the Mismatch Repair Complex Msh2-Msh6. Molecular Cell, 2007, 28, 359-370.	9.7	215
20	Microscopic theory of singlet exciton fission. I. General formulation. Journal of Chemical Physics, 2013, 138, 114102.	3.0	210
21	Local Atomic and Electronic Structure of Boron Chemical Doping in Monolayer Graphene. Nano Letters, 2013, 13, 4659-4665.	9.1	192
22	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
23	Adaptive nudged elastic band approach for transition state calculation. Journal of Chemical Physics, 2002, 117, 4651-4658.	3.0	148
24	Transient superconductivity from electronic squeezing of optically pumped phonons. Nature Physics, 2017, 13, 479-483.	16.7	139
25	Taming the Dynamical Sign Problem in Real-Time Evolution of Quantum Many-Body Problems. Physical Review Letters, 2015, 115, 266802.	7.8	138
26	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
27	Length-Dependent Conductance of Oligothiophenes. Journal of the American Chemical Society, 2014, 136, 10486-10492.	13.7	127
28	Growing Point-to-Set Length Scale Correlates with Growing Relaxation Times in Model Supercooled Liquids. Physical Review Letters, 2012, 108, 225506.	7.8	126
29	Multiphonon Relaxation Slows Singlet Fission in Crystalline Hexacene. Journal of the American Chemical Society, 2014, 136, 10654-10660.	13.7	114
30	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
31	Accurate Force Field Development for Modeling Conjugated Polymers. Journal of Chemical Theory and Computation, 2012, 8, 4556-4569.	5.3	109
32	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
33	How Lattice and Charge Fluctuations Control Carrier Dynamics in Halide Perovskites. Nano Letters, 2018, 18, 8041-8046.	9.1	97
34	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
35	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
36	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

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37	Segregation of Sublattice Domains in Nitrogen-Doped Graphene. Journal of the American Chemical Society, 2014, 136, 1391-1397.	13.7	86
38	Quantum fluctuations can promote or inhibit glassÂformation. Nature Physics, 2011, 7, 134-137.	16.7	84
39	Unbiasing fermionic quantum Monte Carlo with a quantum computer. Nature, 2022, 603, 416-420.	27.8	84
40	Localized soft modes and the supercooled liquidâ€™s irreversible passage through its configuration space. Journal of Chemical Physics, 2009, 131, 194508.	3.0	83
41	Correlation of Local Order with Particle Mobility in Supercooled Liquids Is Highly System Dependent. Physical Review Letters, 2014, 113, 157801.	7.8	83
42	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
43	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
44	The Significance of Polarons and Dynamic Disorder in Halide Perovskites. ACS Energy Letters, 2021, 6, 2162-2173.	17.4	74
45	Cooperativity beyond Caging: Generalized Mode-Coupling Theory. Physical Review Letters, 2006, 97, 095702.	7.8	72
46	Effect of flexibility on hydrophobic behavior of nanotube water channels. Journal of Chemical Physics, 2005, 123, 194502.	3.0	71
47	Transport in quasiperiodic interacting systems: From superdiffusion to subdiffusion. Europhysics Letters, 2017, 119, 37003.	2.0	70
48	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
49	Optical and Excitonic Properties of Atomically Thin Transition-Metal Dichalcogenides. Annual Review of Condensed Matter Physics, 2018, 9, 379-396.	14.5	68
50	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
51	Microscopic Dynamics of Supercooled Liquids from First Principles. Physical Review Letters, 2015, 115, 205701.	7.8	62
52	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
53	Self-Consistent Mode-Coupling Theory for Self-Diffusion in Quantum Liquids. Physical Review Letters, 2001, 87, 265702.	7.8	61
54	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

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55	Impact of Molecular Symmetry on Single-Molecule Conductance. Journal of the American Chemical Society, 2013, 135, 11724-11727.	13.7	57
56	Single-crystal-to-single-crystal intercalation of a low-bandgap superatomic crystal. Nature Chemistry, 2017, 9, 1170-1174.	13.6	56
57	Atomistic Interrogation of Bâ€“N Co-dopant Structures and Their Electronic Effects in Graphene. ACS Nano, 2016, 10, 6574-6584.	14.6	53
58	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
59	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
60	Controlling Chain Conformation in Conjugated Polymers Using Defect Inclusion Strategies. Journal of the American Chemical Society, 2011, 133, 10155-10160.	13.7	52
61	Slow dynamics in a two-dimensional Anderson-Hubbard model. Europhysics Letters, 2016, 113, 46001.	2.0	52
62	On the relaxation of a twoâ€level system: Beyond the weakâ€coupling approximation. Journal of Chemical Physics, 1996, 104, 1506-1518.	3.0	49
63	Comparison of Dynamical Heterogeneity in Hard-Sphere and Attractive Glass Formersâ€. Journal of Physical Chemistry B, 2005, 109, 14654-14658.	2.6	49
64	Time-dependent variational principle in matrix-product state manifolds: Pitfalls and potential. Physical Review B, 2018, 97, .	3.2	49
65	Approximate but accurate quantum dynamics from the Mori formalism: I. Nonequilibrium dynamics. Journal of Chemical Physics, 2016, 144, 184104.	3.0	48
66	A fully self-consistent treatment of collective fluctuations in quantum liquids. Journal of Chemical Physics, 2004, 120, 1458-1465.	3.0	47
67	Depletion of Two-Level Systems in Ultrastable Computer-Generated Glasses. Physical Review Letters, 2020, 124, 225901.	7.8	47
68	Removing instabilities in the hierarchical equations of motion: Exact and approximate projection approaches. Journal of Chemical Physics, 2019, 150, 184109.	3.0	46
69	Classical mapping approaches for nonadiabatic dynamics: Short time analysis. Journal of Chemical Physics, 2001, 114, 1065-1074.	3.0	45
70	Contribution of Slow Clusters to the Bulk Elasticity Near the Colloidal Glass Transition. Physical Review Letters, 2006, 97, 265701.	7.8	45
71	On the accuracy of surface hopping dynamics in condensed phase non-adiabatic problems. Journal of Chemical Physics, 2016, 144, 094104.	3.0	43
72	Molecular Engineering of Chromophores to Enable Tripletâ€“Triplet Annihilation Upconversion. Journal of the American Chemical Society, 2020, 142, 19917-19925.	13.7	42

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73	Extending the applicability of Redfield theories into highly non-Markovian regimes. Journal of Chemical Physics, 2015, 143, 194108.	3.0	41
74	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
75	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
76	Phaseless Auxiliary-Field Quantum Monte Carlo on Graphical Processing Units. Journal of Chemical Theory and Computation, 2018, 14, 4109-4121.	5.3	35
77	Multiset Matrix Product State Calculations Reveal Mobile Franck-Condon Excitations Under Strong Holstein-Type Coupling. Physical Review Letters, 2019, 123, 126601.	7.8	35
78	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
79	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
80	Equilibrium ultrastable glasses produced by random pinning. Journal of Chemical Physics, 2014, 141, 224503.	3.0	31
81	Cumulant expansions and the spin-boson problem. Physical Review E, 1997, 55, 2328-2337.	2.1	30
82	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
83	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
84	On the nonperturbative theory of pure dephasing in condensed phases at low temperatures. Journal of Chemical Physics, 1996, 105, 10500-10506.	3.0	28
85	Numerical Investigation of the Entropy Crisis in Model Glass Formers. Journal of Physical Chemistry B, 2004, 108, 6832-6837.	2.6	28
86	Many-body theory of optical absorption in doped two-dimensional semiconductors. Physical Review B, 2019, 99, .	3.2	28
87	Analytic continuation for quantum nonadiabatic rate constants. Journal of Chemical Physics, 2003, 118, 457-460.	3.0	27
88	Numerical Investigation of Glassy Dynamics in Low-Density Systems. Physical Review Letters, 2008, 100, 195701.	7.8	27
89	A Short-Time Quantum Mechanical Expansion Approach to Vibrational Relaxationâ€. Journal of Physical Chemistry B, 2001, 105, 6550-6555.	2.6	26
90	Molecular hydrodynamic theory of nonresonant Raman spectra in liquids: Fifth-order spectra. Journal of Chemical Physics, 2002, 116, 1987-1994.	3.0	24

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91	On the multiple time scales in solvation dynamics: A mode-coupling theory approach. Journal of Chemical Physics, 2002, 116, 5080.	3.0	24
92	Nonequilibrium transport in quantum impurity models: exact path integral simulations. Physical Chemistry Chemical Physics, 2011, 13, 14378.	2.8	24
93	Chromophore-Controlled Self-Assembly of Highly Ordered Polymer Nanostructures. Journal of Physical Chemistry Letters, 2013, 4, 2520-2524.	4.6	22
94	Spectral diffusion on ultralong time scales in low-temperature glasses. Physical Review B, 1997, 56, 5250-5260.	3.2	21
95	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
96	Transport properties of normal liquid helium: Comparison of various methodologies. Journal of Chemical Physics, 2005, 123, 184506.	3.0	18
97	On the accuracy of the PadÃ©-resummed master equation approach to dissipative quantum dynamics. Journal of Chemical Physics, 2016, 144, 154106.	3.0	17
98	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
99	Molecular hydrodynamic theory of nonresonant Raman spectra in liquids: Third-order spectra. Journal of Chemical Physics, 2002, 116, 1979-1986.	3.0	16
100	The Subdiffusive Targeting Problem. Journal of Physical Chemistry B, 2008, 112, 4283-4289.	2.6	16
101	Generalization of fewest-switches surface hopping for coherences. Journal of Chemical Physics, 2018, 148, 102309.	3.0	15
102	Interlayer Excitons in Transitionâ€Metal Dichalcogenide Heterobilayers. Physica Status Solidi (B): Basic Research, 2019, 256, 1900308.	1.5	15
103	Stochastic resolution-of-the-identity auxiliary-field quantum Monte Carlo: Scaling reduction without overhead. Journal of Chemical Physics, 2020, 153, 044131.	3.0	15
104	Microscopic model of the doping dependence of linewidths in monolayer transition metal dichalcogenides. Journal of Chemical Physics, 2020, 152, 194705.	3.0	15
105	Superatomic solid solutions. Nature Chemistry, 2021, 13, 607-613.	13.6	15
106	Critical tests of a new master equation approach to nonadiabatic quantum dissipative systems. Chemical Physics, 2004, 296, 129-134.	1.9	13
107	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
108	Critical Dynamical Heterogeneities Close to Continuous Second-Order Glass Transitions. Physical Review Letters, 2014, 113, 245701.	7.8	13

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109	On mean-field theories of dynamics in supercooled liquids. Journal of Chemical Physics, 2019, 151, 084503.	3.0	13
110	Studying dynamics in two-dimensional quantum lattices using tree tensor network states. SciPost Physics, 2020, 9, .	4.9	13
111	Semiclassical representations of electronic structure and dynamics. Journal of Chemical Physics, 2004, 120, 579-589.	3.0	10
112	Relationship between Mechanical and Dynamical Properties of Glass Forming Liquidsâ€. Journal of Physical Chemistry B, 2004, 108, 19703-19710.	2.6	10
113	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
114	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
115	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
116	Time evolution of ML-MCTDH wavefunctions. I. Gauge conditions, basis functions, and singularities. Journal of Chemical Physics, 2021, 155, 174108.	3.0	7
117	A Localized-Orbital Energy Evaluation for Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2022, 18, 3447-3459.	5.3	7
118	Calculating approximate quantum mechanical rates without an a priori reaction coordinate. Journal of Chemical Physics, 2002, 116, 8376.	3.0	6
119	Analytic continuation average spectrum method for transport in quantum liquids. Chemical Physics, 2010, 370, 132-136.	1.9	6
120	On Stochastic Models of Dynamic Disorderâ€. Journal of Physical Chemistry B, 2006, 110, 19061-19065.	2.6	5
121	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
122	Time evolution of ML-MCTDH wavefunctions. II. Application of the projector splitting integrator. Journal of Chemical Physics, 2021, 155, 174109.	3.0	5
123	Cumulant methods for electron-phonon problems. I. Perturbative expansions. Physical Review B, 2022, 105, .	3.2	5
124	Self-consistent harmonic theory of solvation in glassy systems: Classical solvation. Journal of Chemical Physics, 2000, 112, 3267-3279.	3.0	4
125	Self-consistent harmonic theory of solvation in glassy systems: Quantum solvation. Journal of Chemical Physics, 2000, 112, 3280-3284.	3.0	3
126	Singlet fission. Journal of Chemical Physics, 2020, 153, 110401.	3.0	3

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127	Alternative model of dissipation in quantum mechanics. Physical Review E, 1996, 53, 4184-4186.	2.1	2
128	JCP Emerging Investigator Special Collection 2019. Journal of Chemical Physics, 2020, 153, 110402.	3.0	2
129	2D materials. Journal of Chemical Physics, 2021, 154, 040401.	3.0	1
130	Strongly Correlated Ladders in K-Doped p-Terphenyl Crystals. Nano Letters, 2021, 21, 9573-9579.	9.1	1
131	2020 JCP Emerging Investigator Special Collection. Journal of Chemical Physics, 2021, 155, 230401.	3.0	1
132	Tribute to Robert J. Silbey. Journal of Physical Chemistry B, 2006, 110, 18734-18734.	2.6	0
133	E. Coli RNA Polymerase Searches for Promoters through 3D Diffusion. Biophysical Journal, 2013, 104, 541a.	0.5	0
134	Chemical physics of materials. Journal of Chemical Physics, 2020, 153, 100402.	3.0	0