

David R Reichman

List of Publications by Year in descending order

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134
papers

15,901
citations

34493

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17891

125
g-index

135
all docs

135
docs citations

135
times ranked

21891
citing authors

#	ARTICLE	IF	CITATIONS
1	Unbiasing fermionic quantum Monte Carlo with a quantum computer. <i>Nature</i> , 2022, 603, 416-420.	13.7	84
2	A Localized-Orbital Energy Evaluation for Auxiliary-Field Quantum Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3447-3459.	2.3	7
3	Cumulant methods for electron-phonon problems. I. Perturbative expansions. <i>Physical Review B</i> , 2022, 105, .	1.1	5
4	2D materials. <i>Journal of Chemical Physics</i> , 2021, 154, 040401.	1.2	1
5	Superatomic solid solutions. <i>Nature Chemistry</i> , 2021, 13, 607-613.	6.6	15
6	Spectral Functions from Auxiliary-Field Quantum Monte Carlo without Analytic Continuation: The Extended Koopmans's™ Theorem Approach. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3372-3387.	2.3	10
7	The Significance of Polarons and Dynamic Disorder in Halide Perovskites. <i>ACS Energy Letters</i> , 2021, 6, 2162-2173.	8.8	74
8	Time evolution of ML-MCTDH wavefunctions. II. Application of the projector splitting integrator. <i>Journal of Chemical Physics</i> , 2021, 155, 174109.	1.2	5
9	Time evolution of ML-MCTDH wavefunctions. I. Gauge conditions, basis functions, and singularities. <i>Journal of Chemical Physics</i> , 2021, 155, 174108.	1.2	7
10	Strongly Correlated Ladders in K-Doped p-Terphenyl Crystals. <i>Nano Letters</i> , 2021, 21, 9573-9579.	4.5	1
11	2020 JCP Emerging Investigator Special Collection. <i>Journal of Chemical Physics</i> , 2021, 155, 230401.	1.2	1
12	JCP Emerging Investigator Special Collection 2019. <i>Journal of Chemical Physics</i> , 2020, 153, 110402.	1.2	2
13	Molecular Engineering of Chromophores to Enable Triplet-Triplet Annihilation Upconversion. <i>Journal of the American Chemical Society</i> , 2020, 142, 19917-19925.	6.6	42
14	Singlet fission. <i>Journal of Chemical Physics</i> , 2020, 153, 110401.	1.2	3
15	Chemical physics of materials. <i>Journal of Chemical Physics</i> , 2020, 153, 100402.	1.2	0
16	Stochastic resolution-of-the-identity auxiliary-field quantum Monte Carlo: Scaling reduction without overhead. <i>Journal of Chemical Physics</i> , 2020, 153, 044131.	1.2	15
17	The performance of phaseless auxiliary-field quantum Monte Carlo on the ground state electronic energy of benzene. <i>Journal of Chemical Physics</i> , 2020, 153, 126101.	1.2	17
18	Depletion of Two-Level Systems in Ultrastable Computer-Generated Glasses. <i>Physical Review Letters</i> , 2020, 124, 225901.	2.9	47

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19	Multiple Stable Isoprene-Ozone Complexes Reveal Complex Entrance Channel Dynamics in the Isoprene + Ozone Reaction. <i>Journal of the American Chemical Society</i> , 2020, 142, 10806-10813.	6.6	9
20	Microscopic model of the doping dependence of linewidths in monolayer transition metal dichalcogenides. <i>Journal of Chemical Physics</i> , 2020, 152, 194705.	1.2	15
21	Predicting Ligand-Dissociation Energies of 3d Coordination Complexes with Auxiliary-Field Quantum Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3041-3054.	2.3	21
22	Studying dynamics in two-dimensional quantum lattices using tree tensor network states. <i>SciPost Physics</i> , 2020, 9, .	1.5	13
23	Singlet-Triplet Energy Gaps of Organic Biradicals and Polyacenes with Auxiliary-Field Quantum Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4924-4932.	2.3	37
24	Perylene Diimide-Based H _v - and h _v -Aggregates: The Prospect of Exciton Band Shape Engineering in Organic Materials. <i>Journal of Physical Chemistry C</i> , 2019, 123, 20567-20578.	1.5	91
25	Removing instabilities in the hierarchical equations of motion: Exact and approximate projection approaches. <i>Journal of Chemical Physics</i> , 2019, 150, 184109.	1.2	46
26	Interlayer Excitons in Transition-Metal Dichalcogenide Heterobilayers. <i>Physica Status Solidi (B): Basic Research</i> , 2019, 256, 1900308.	0.7	15
27	Multiset Matrix Product State Calculations Reveal Mobile Franck-Condon Excitations Under Strong Holstein-Type Coupling. <i>Physical Review Letters</i> , 2019, 123, 126601.	2.9	35
28	On mean-field theories of dynamics in supercooled liquids. <i>Journal of Chemical Physics</i> , 2019, 151, 084503.	1.2	13
29	On Achieving High Accuracy in Quantum Chemical Calculations of 3<i>d</i> Transition Metal-Containing Systems: A Comparison of Auxiliary-Field Quantum Monte Carlo with Coupled Cluster, Density Functional Theory, and Experiment for Diatomic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2346-2358.	2.3	62
30	Many-body theory of optical absorption in doped two-dimensional semiconductors. <i>Physical Review B</i> , 2019, 99, .	1.1	28
31	Time-dependent variational principle in matrix-product state manifolds: Pitfalls and potential. <i>Physical Review B</i> , 2018, 97, .	1.1	49
32	Optical and Excitonic Properties of Atomically Thin Transition-Metal Dichalcogenides. <i>Annual Review of Condensed Matter Physics</i> , 2018, 9, 379-396.	5.2	68
33	Generalization of fewest-switches surface hopping for coherences. <i>Journal of Chemical Physics</i> , 2018, 148, 102309.	1.2	15
34	Momentum-space indirect interlayer excitons in transition-metal dichalcogenide van der Waals heterostructures. <i>Nature Physics</i> , 2018, 14, 801-805.	6.5	229
35	How Lattice and Charge Fluctuations Control Carrier Dynamics in Halide Perovskites. <i>Nano Letters</i> , 2018, 18, 8041-8046.	4.5	97
36	Vibronic exciton theory of singlet fission. III. How vibronic coupling and thermodynamics promote rapid triplet generation in pentacene crystals. <i>Journal of Chemical Physics</i> , 2018, 148, 244701.	1.2	67

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37	Phaseless Auxiliary-Field Quantum Monte Carlo on Graphical Processing Units. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4109-4121.	2.3	35
38	Transient superconductivity from electronic squeezing of optically pumped phonons. <i>Nature Physics</i> , 2017, 13, 479-483.	6.5	139
39	Vibronic exciton theory of singlet fission. II. Two-dimensional spectroscopic detection of the correlated triplet pair state. <i>Journal of Chemical Physics</i> , 2017, 146, 174704.	1.2	53
40	Vibronic exciton theory of singlet fission. I. Linear absorption and the anatomy of the correlated triplet pair state. <i>Journal of Chemical Physics</i> , 2017, 146, 174703.	1.2	77
41	Chemical Transformations Approaching Chemical Accuracy via Correlated Sampling in Auxiliary-Field Quantum Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2667-2680.	2.3	33
42	Triplet Separation Drives Singlet Fission after Femtosecond Correlated Triplet Pair Production in Rubrene. <i>Journal of the American Chemical Society</i> , 2017, 139, 11745-11751.	6.6	107
43	Single-crystal-to-single-crystal intercalation of a low-bandgap superatomic crystal. <i>Nature Chemistry</i> , 2017, 9, 1170-1174.	6.6	56
44	Transport in quasiperiodic interacting systems: From superdiffusion to subdiffusion. <i>Europhysics Letters</i> , 2017, 119, 37003.	0.7	70
45	Slow dynamics in a two-dimensional Anderson-Hubbard model. <i>Europhysics Letters</i> , 2016, 113, 46001.	0.7	52
46	On the accuracy of surface hopping dynamics in condensed phase non-adiabatic problems. <i>Journal of Chemical Physics</i> , 2016, 144, 094104.	1.2	43
47	On the accuracy of the Pad�-resummed master equation approach to dissipative quantum dynamics. <i>Journal of Chemical Physics</i> , 2016, 144, 154106.	1.2	17
48	Approximate but accurate quantum dynamics from the Mori formalism: I. Nonequilibrium dynamics. <i>Journal of Chemical Physics</i> , 2016, 144, 184104.	1.2	48
49	Atomistic Interrogation of ¹⁵ N Co-dopant Structures and Their Electronic Effects in Graphene. <i>ACS Nano</i> , 2016, 10, 6574-6584.	7.3	53
50	Energy Transfer from Quantum Dots to Graphene and MoS ₂ : The Role of Absorption and Screening in Two-Dimensional Materials. <i>Nano Letters</i> , 2016, 16, 2328-2333.	4.5	179
51	Algorithm independent bounds on community detection problems and associated transitions in stochastic block model graphs. <i>Journal of Complex Networks</i> , 2015, 3, 333-360.	1.1	5
52	Microscopic Dynamics of Supercooled Liquids from First Principles. <i>Physical Review Letters</i> , 2015, 115, 205701.	2.9	62
53	Taming the Dynamical Sign Problem in Real-Time Evolution of Quantum Many-Body Problems. <i>Physical Review Letters</i> , 2015, 115, 266802.	2.9	138
54	Extending the applicability of Redfield theories into highly non-Markovian regimes. <i>Journal of Chemical Physics</i> , 2015, 143, 194108.	1.2	41

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55	Absence of Diffusion in an Interacting System of Spinless Fermions on a One-Dimensional Disordered Lattice. <i>Physical Review Letters</i> , 2015, 114, 100601.	2.9	246
56	Observation of biexcitons in monolayer WSe ₂ . <i>Nature Physics</i> , 2015, 11, 477-481.	6.5	531
57	Observation of Excitonic Rydberg States in Monolayer MoS ₂ and WS ₂ by Photoluminescence Excitation Spectroscopy. <i>Nano Letters</i> , 2015, 15, 2992-2997.	4.5	327
58	Critical Dynamical Heterogeneities Close to Continuous Second-Order Glass Transitions. <i>Physical Review Letters</i> , 2014, 113, 245701.	2.9	13
59	Equilibrium ultrastable glasses produced by random pinning. <i>Journal of Chemical Physics</i> , 2014, 141, 224503.	1.2	31
60	Greenâ€™s Functions from Real-Time Bold-Line Monteâ€™Carlo Calculations: Spectral Properties of the Nonequilibrium Anderson Impurity Model. <i>Physical Review Letters</i> , 2014, 112, 146802.	2.9	80
61	Segregation of Sublattice Domains in Nitrogen-Doped Graphene. <i>Journal of the American Chemical Society</i> , 2014, 136, 1391-1397.	6.6	86
62	Correlation of Local Order with Particle Mobility in Supercooled Liquids Is Highly System Dependent. <i>Physical Review Letters</i> , 2014, 113, 157801.	2.9	83
63	Multiphonon Relaxation Slows Singlet Fission in Crystalline Hexacene. <i>Journal of the American Chemical Society</i> , 2014, 136, 10654-10660.	6.6	114
64	Length-Dependent Conductance of Oligothiophenes. <i>Journal of the American Chemical Society</i> , 2014, 136, 10486-10492.	6.6	127
65	Exciton Binding Energy and Nonhydrogenic Rydberg Series in Monolayer WS_2 . <i>Physical Review Letters</i> , 2014, 113, 076802.	2.9	1,814
66	Tailoring the Electronic Structure in Bilayer Molybdenum Disulfide via Interlayer Twist. <i>Nano Letters</i> , 2014, 14, 3869-3875.	4.5	278
67	Impact of Molecular Symmetry on Single-Molecule Conductance. <i>Journal of the American Chemical Society</i> , 2013, 135, 11724-11727.	6.6	57
68	Chromophore-Controlled Self-Assembly of Highly Ordered Polymer Nanostructures. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2520-2524.	2.1	22
69	Theory of neutral and charged excitons in monolayer transition metal dichalcogenides. <i>Physical Review B</i> , 2013, 88, .	1.1	737
70	Local Atomic and Electronic Structure of Boron Chemical Doping in Monolayer Graphene. <i>Nano Letters</i> , 2013, 13, 4659-4665.	4.5	192
71	Coherent quantum dynamics in donorâ€™bridgeâ€™acceptor systems: beyond the hopping and super-exchange mechanisms. <i>New Journal of Physics</i> , 2013, 15, 105020.	1.2	30
72	Microscopic theory of singlet exciton fission. II. Application to pentacene dimers and the role of superexchange. <i>Journal of Chemical Physics</i> , 2013, 138, 114103.	1.2	311

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73	The promoter-search mechanism of Escherichia coli RNA polymerase is dominated by three-dimensional diffusion. <i>Nature Structural and Molecular Biology</i> , 2013, 20, 174-181.	3.6	110
74	Dynamic Length Scales in Glass-Forming Liquids: An Inhomogeneous Molecular Dynamics Simulation Approach. <i>Journal of Physical Chemistry B</i> , 2013, 117, 13259-13267.	1.2	7
75	E. Coli RNA Polymerase Searches for Promoters through 3D Diffusion. <i>Biophysical Journal</i> , 2013, 104, 541a.	0.2	0
76	The Quantum Coherent Mechanism for Singlet Fission: Experiment and Theory. <i>Accounts of Chemical Research</i> , 2013, 46, 1321-1329.	7.6	262
77	Microscopic theory of singlet exciton fission. I. General formulation. <i>Journal of Chemical Physics</i> , 2013, 138, 114102.	1.2	210
78	Grains and grain boundaries in highly crystalline monolayer molybdenum disulphide. <i>Nature Materials</i> , 2013, 12, 554-561.	13.3	1,896
79	A small subset of normal modes mimics the properties of dynamical heterogeneity in a model supercooled liquid. <i>Journal of Chemical Physics</i> , 2013, 138, 12A537.	1.2	13
80	Accurate Force Field Development for Modeling Conjugated Polymers. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4556-4569.	2.3	109
81	Connecting Dopant Bond Type with Electronic Structure in N-Doped Graphene. <i>Nano Letters</i> , 2012, 12, 4025-4031.	4.5	471
82	Growing Point-to-Set Length Scale Correlates with Growing Relaxation Times in Model Supercooled Liquids. <i>Physical Review Letters</i> , 2012, 108, 225506.	2.9	126
83	Nonequilibrium transport in quantum impurity models: exact path integral simulations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14378.	1.3	24
84	Visualizing Individual Nitrogen Dopants in Monolayer Graphene. <i>Science</i> , 2011, 333, 999-1003.	6.0	774
85	Quantum fluctuations can promote or inhibit glass formation. <i>Nature Physics</i> , 2011, 7, 134-137.	6.5	84
86	Controlling Chain Conformation in Conjugated Polymers Using Defect Inclusion Strategies. <i>Journal of the American Chemical Society</i> , 2011, 133, 10155-10160.	6.6	52
87	Analytic continuation average spectrum method for transport in quantum liquids. <i>Chemical Physics</i> , 2010, 370, 132-136.	0.9	6
88	Spatial dimension and the dynamics of supercooled liquids. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 15171-15175.	3.3	68
89	Localized soft modes and the supercooled liquid's irreversible passage through its configuration space. <i>Journal of Chemical Physics</i> , 2009, 131, 194508.	1.2	83
90	Soft colloids make strong glasses. <i>Nature</i> , 2009, 462, 83-86.	13.7	464

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91	Irreversible reorganization in a supercooled liquid originates from localized soft modes. <i>Nature Physics</i> , 2008, 4, 711-715.	6.5	367
92	The Subdiffusive Targeting Problem. <i>Journal of Physical Chemistry B</i> , 2008, 112, 4283-4289.	1.2	16
93	Numerical Investigation of Glassy Dynamics in Low-Density Systems. <i>Physical Review Letters</i> , 2008, 100, 195701.	2.9	27
94	Dynamic Basis for One-Dimensional DNA Scanning by the Mismatch Repair Complex Msh2-Msh6. <i>Molecular Cell</i> , 2007, 28, 359-370.	4.5	215
95	Strain-Rate Frequency Superposition: A Rheological Probe of Structural Relaxation in Soft Materials. <i>Physical Review Letters</i> , 2007, 98, 238303.	2.9	220
96	Inhomogeneous Mode-Coupling Theory and Growing Dynamic Length in Supercooled Liquids. <i>Physical Review Letters</i> , 2006, 97, 195701.	2.9	262
97	On Stochastic Models of Dynamic Disorder. <i>Journal of Physical Chemistry B</i> , 2006, 110, 19061-19065.	1.2	5
98	Tribute to Robert J. Silbey. <i>Journal of Physical Chemistry B</i> , 2006, 110, 18734-18734.	1.2	0
99	Cooperativity beyond Caging: Generalized Mode-Coupling Theory. <i>Physical Review Letters</i> , 2006, 97, 095702.	2.9	72
100	Contribution of Slow Clusters to the Bulk Elasticity Near the Colloidal Glass Transition. <i>Physical Review Letters</i> , 2006, 97, 265701.	2.9	45
101	QUANTUM MODE-COUPPLING THEORY: Formulation and Applications to Normal and Supercooled Quantum Liquids. <i>Annual Review of Physical Chemistry</i> , 2005, 56, 157-185.	4.8	33
102	Magnetic self-assembly of three-dimensional surfaces from planar sheets. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 3924-3929.	3.3	131
103	Transport properties of normal liquid helium: Comparison of various methodologies. <i>Journal of Chemical Physics</i> , 2005, 123, 184506.	1.2	18
104	Mode-coupling theory. <i>Journal of Statistical Mechanics: Theory and Experiment</i> , 2005, 2005, P05013.	0.9	228
105	Comparison of Dynamical Heterogeneity in Hard-Sphere and Attractive Glass Formers. <i>Journal of Physical Chemistry B</i> , 2005, 109, 14654-14658.	1.2	49
106	Effect of flexibility on hydrophobic behavior of nanotube water channels. <i>Journal of Chemical Physics</i> , 2005, 123, 194502.	1.2	71
107	Semiclassical representations of electronic structure and dynamics. <i>Journal of Chemical Physics</i> , 2004, 120, 579-589.	1.2	10
108	A fully self-consistent treatment of collective fluctuations in quantum liquids. <i>Journal of Chemical Physics</i> , 2004, 120, 1458-1465.	1.2	47

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109	Critical tests of a new master equation approach to nonadiabatic quantum dissipative systems. <i>Chemical Physics</i> , 2004, 296, 129-134.	0.9	13
110	Relationship between Mechanical and Dynamical Properties of Glass Forming Liquids. <i>Journal of Physical Chemistry B</i> , 2004, 108, 19703-19710.	1.2	10
111	Numerical Investigation of the Entropy Crisis in Model Glass Formers. <i>Journal of Physical Chemistry B</i> , 2004, 108, 6832-6837.	1.2	28
112	Drying-mediated self-assembly of nanoparticles. <i>Nature</i> , 2003, 426, 271-274.	13.7	866
113	Analytic continuation for quantum nonadiabatic rate constants. <i>Journal of Chemical Physics</i> , 2003, 118, 457-460.	1.2	27
114	Molecular hydrodynamic theory of nonresonant Raman spectra in liquids: Third-order spectra. <i>Journal of Chemical Physics</i> , 2002, 116, 1979-1986.	1.2	16
115	A self-consistent mode-coupling theory for dynamical correlations in quantum liquids: Application to liquid para-hydrogen. <i>Journal of Chemical Physics</i> , 2002, 116, 6279-6285.	1.2	60
116	Molecular hydrodynamic theory of nonresonant Raman spectra in liquids: Fifth-order spectra. <i>Journal of Chemical Physics</i> , 2002, 116, 1987-1994.	1.2	24
117	Adaptive nudged elastic band approach for transition state calculation. <i>Journal of Chemical Physics</i> , 2002, 117, 4651-4658.	1.2	148
118	A self-consistent mode-coupling theory for dynamical correlations in quantum liquids: Rigorous formulation. <i>Journal of Chemical Physics</i> , 2002, 116, 6271-6278.	1.2	52
119	Calculating approximate quantum mechanical rates without an a priori reaction coordinate. <i>Journal of Chemical Physics</i> , 2002, 116, 8376.	1.2	6
120	The calculation of transport properties in quantum liquids using the maximum entropy numerical analytic continuation method: Application to liquid para-hydrogen. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 1129-1133.	3.3	89
121	On the multiple time scales in solvation dynamics: A mode-coupling theory approach. <i>Journal of Chemical Physics</i> , 2002, 116, 5080.	1.2	24
122	Self-Consistent Mode-Coupling Theory for Self-Diffusion in Quantum Liquids. <i>Physical Review Letters</i> , 2001, 87, 265702.	2.9	61
123	Reference system master equation approaches to condensed phase charge transfer processes. I. General formulation. <i>Journal of Chemical Physics</i> , 2001, 115, 9848-9861.	1.2	39
124	A Short-Time Quantum Mechanical Expansion Approach to Vibrational Relaxation. <i>Journal of Physical Chemistry B</i> , 2001, 105, 6550-6555.	1.2	26
125	Classical mapping approaches for nonadiabatic dynamics: Short time analysis. <i>Journal of Chemical Physics</i> , 2001, 114, 1065-1074.	1.2	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. <i>Journal of Chemical Physics</i> , 2001, 115, 9862-9870.	1.2	29

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127	A Feynman path centroid dynamics approach for the computation of time correlation functions involving nonlinear operators. <i>Journal of Chemical Physics</i> , 2000, 113, 919-929.	1.2	91
128	Self-consistent harmonic theory of solvation in glassy systems: Quantum solvation. <i>Journal of Chemical Physics</i> , 2000, 112, 3280-3284.	1.2	3
129	Self-consistent harmonic theory of solvation in glassy systems: Classical solvation. <i>Journal of Chemical Physics</i> , 2000, 112, 3267-3279.	1.2	4
130	Spectral diffusion on ultralong time scales in low-temperature glasses. <i>Physical Review B</i> , 1997, 56, 5250-5260.	1.1	21
131	Cumulant expansions and the spin-boson problem. <i>Physical Review E</i> , 1997, 55, 2328-2337.	0.8	30
132	On the relaxation of a two-level system: Beyond the weak-coupling approximation. <i>Journal of Chemical Physics</i> , 1996, 104, 1506-1518.	1.2	49
133	On the nonperturbative theory of pure dephasing in condensed phases at low temperatures. <i>Journal of Chemical Physics</i> , 1996, 105, 10500-10506.	1.2	28
134	Alternative model of dissipation in quantum mechanics. <i>Physical Review E</i> , 1996, 53, 4184-4186.	0.8	2