Timothy C Berkelbach

List of Publications by Year
in descending order

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66 papers	10,578 citations	117625 34 h-index	106344 65 g-index
66 all docs	66 docs citations	66 times ranked	11667 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	P<scp>y</scp>SCF: the Pythonâ€based simulations of chemistry framework. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1340.	14.6	894
4	Theory of neutral and charged excitons in monolayer transition metal dichalcogenides. Physical Review B, 2013, 88, .	3.2	737
5	Observation of biexcitons in monolayer WSe2. Nature Physics, 2015, 11, 477-481.	16.7	531
6	Coulomb engineering of the bandgap and excitons in two-dimensional materials. Nature Communications, 2017, 8, 15251.	12.8	526
7	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
8	Observation of Excitonic Rydberg States in Monolayer MoS₂ and WS₂ by Photoluminescence Excitation Spectroscopy. Nano Letters, 2015, 15, 2992-2997.	9.1	327
9	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
10	Tailoring the Electronic Structure in Bilayer Molybdenum Disulfide via Interlayer Twist. Nano Letters, 2014, 14, 3869-3875.	9.1	278
11	The Quantum Coherent Mechanism for Singlet Fission: Experiment and Theory. Accounts of Chemical Research, 2013, 46, 1321-1329.	15.6	262
12	Dielectric disorder in two-dimensional materials. Nature Nanotechnology, 2019, 14, 832-837.	31.5	223
13	Microscopic theory of singlet exciton fission. I. General formulation. Journal of Chemical Physics, 2013, 138, 114102.	3.0	210
14	Concerted Hydrogen-Bond Dynamics in the Transport Mechanism of the Hydrated Proton: A First-Principles Molecular Dynamics Study. Physical Review Letters, 2009, 103, 238302.	7.8	200
15	Gaussian-Based Coupled-Cluster Theory for the Ground-State and Band Structure of Solids. Journal of Chemical Theory and Computation, 2017, 13, 1209-1218.	5.3	171
16	Microscopic theory of singlet exciton fission. III. Crystalline pentacene. Journal of Chemical Physics, 2014, 141, 074705.	3.0	160
17	Length-Dependent Conductance of Oligothiophenes. Journal of the American Chemical Society, 2014, 136, 10486-10492.	13.7	127
18	Multiphonon Relaxation Slows Singlet Fission in Crystalline Hexacene. Journal of the American Chemical Society, 2014, 136, 10654-10660.	13.7	114

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19	Environmentally sensitive theory of electronic and optical transitions in atomically thin semiconductors. Physical Review B, 2018, 97, .	3.2	93
20	Binding energies and spatial structures of small carrier complexes in monolayer transition-metal dichalcogenides via diffusion Monte Carlo. Physical Review B, 2015, 92, .	3.2	88
21	Spectral functions of the uniform electron gas via coupled-cluster theory and comparison to the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mm related approximations. Physical Review B, 2016, 93, .	3.2	70
22	Bright and dark singlet excitons via linear and two-photon spectroscopy in monolayer transition-metal dichalcogenides. Physical Review B, 2015, 92, .	3.2	68
23	Optical and Excitonic Properties of Atomically Thin Transition-Metal Dichalcogenides. Annual Review of Condensed Matter Physics, 2018, 9, 379-396.	14.5	68
24	Gaussian and plane-wave mixed density fitting for periodic systems. Journal of Chemical Physics, 2017, 147, 164119.	3.0	66
25	Reduced density matrix hybrid approach: An efficient and accurate method for adiabatic and non-adiabatic quantum dynamics. Journal of Chemical Physics, 2012, 136, 034113.	3.0	58
26	On the Relation between Equation-of-Motion Coupled-Cluster Theory and the GW Approximation. Journal of Chemical Theory and Computation, 2018, 14, 4224-4236.	5.3	58
27	Reduced density matrix hybrid approach: Application to electronic energy transfer. Journal of Chemical Physics, 2012, 136, 084104.	3.0	57
28	Impact of Molecular Symmetry on Single-Molecule Conductance. Journal of the American Chemical Society, 2013, 135, 11724-11727.	13.7	57
29	Optical Properties of Layered Hybrid Organicâ€“Inorganic Halide Perovskites: A Tight-Binding GW-BSE Study. Journal of Physical Chemistry Letters, 2019, 10, 6189-6196.	4.6	51
30	Many-body simulation of two-dimensional electronic spectroscopy of excitons and trions in monolayer transition metal dichalcogenides. Nature Communications, 2019, 10, 3419.	12.8	46
31	Excitons in Solids from Periodic Equation-of-Motion Coupled-Cluster Theory. Journal of Chemical Theory and Computation, 2020, 16, 3095-3103.	5.3	43
32	Linear and nonlinear spectroscopy from quantum master equations. Journal of Chemical Physics, 2017, 147, 244109.	3.0	42
33	Extending the applicability of Redfield theories into highly non-Markovian regimes. Journal of Chemical Physics, 2015, 143, 194108.	3.0	41
34	Coupled-cluster impurity solvers for dynamical mean-field theory. Physical Review B, 2019, 100, .	3.2	37
35	Regional Embedding Enables High-Level Quantum Chemistry for Surface Science. Journal of Physical Chemistry Letters, 2021, 12, 1104-1109.	4.6	33
36	Full-frequency GW without frequency. Journal of Chemical Physics, 2021, 154, 041101.	3.0	32

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37	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
38	A Unification of the Holstein Polaron and Dynamic Disorder Pictures of Charge Transport in Organic Crystals. Physical Review X, 2020, 10, .	8.9	30
39	Tunable Cr⁴⁺ Molecular Color Centers. Journal of the American Chemical Society, 2021, 143, 21350-21363.	13.7	29
40	Quantum quench spectroscopy of a Luttinger liquid: Ultrarelativistic density wave dynamics due to fractionalization in anXXZchain. Physical Review B, 2011, 84, .	3.2	21
41	Vertex Corrections to the Polarizability Do Not Improve the GW Approximation for the Ionization Potential of Molecules. Journal of Chemical Theory and Computation, 2019, 15, 2925-2932.	5.3	21
42	Correlation-Consistent Gaussian Basis Sets for Solids Made Simple. Journal of Chemical Theory and Computation, 2022, 18, 1595-1606.	5.3	19
43	Beyond Walkers in Stochastic Quantum Chemistry: Reducing Error Using Fast Randomized Iteration. Journal of Chemical Theory and Computation, 2019, 15, 4834-4850.	5.3	18
44	On the accuracy of the PadÃ©-resummed master equation approach to dissipative quantum dynamics. Journal of Chemical Physics, 2016, 144, 154106.	3.0	17
45	Communication: Random-phase approximation excitation energies from approximate equation-of-motion coupled-cluster doubles. Journal of Chemical Physics, 2018, 149, 041103.	3.0	17
46	Fast periodic Gaussian density fitting by range separation. Journal of Chemical Physics, 2021, 154, 131104.	3.0	17
47	Dark-Exciton Driven Energy Funneling into Dielectric Inhomogeneities in Two-Dimensional Semiconductors. Nano Letters, 2022, 22, 2843-2850.	9.1	17
48	Large Band Edge Tunability in Colloidal Nanoplatelets. Nano Letters, 2019, 19, 7124-7129.	9.1	15
49	AbÂInitio Lifetime and Concomitant Double-Excitation Character of Plasmons at Metallic Densities. Physical Review Letters, 2019, 122, 226402.	7.8	15
50	Vibrational heat-bath configuration interaction. Journal of Chemical Physics, 2021, 154, 074104.	3.0	14
51	Dynamical correlation energy of metals in large basis sets from downfolding and composite approaches. Journal of Chemical Physics, 2021, 154, 211105.	3.0	13
52	Absorption Spectra of Solids from Periodic Equation-of-Motion Coupled-Cluster Theory. Journal of Chemical Theory and Computation, 2021, 17, 6387-6394.	5.3	13
53	Full-frequency dynamical Betheâ€“Salpeter equation without frequency and a study of double excitations. Journal of Chemical Physics, 2022, 156, 044114.	3.0	11
54	Active space approaches combining coupled-cluster and perturbation theory for ground states and excited states. Molecular Physics, 2020, 118, e1808726.	1.7	9

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55	Simulations of Trions and Biexcitons in Layered Hybrid Organic-Inorganic Lead Halide Perovskites. Physical Review Letters, 2021, 126, 216402.	7.8	9
56	Tight distance-dependent estimators for screening two-center and three-center short-range Coulomb integrals over Gaussian basis functions. Journal of Chemical Physics, 2021, 155, 124106.	3.0	9
57	Optimizing the switching function for nonequilibrium free-energy calculations: An on-the-fly approach. Journal of Chemical Physics, 2009, 130, 174705.	3.0	8
58	Improved Fast Randomized Iteration Approach to Full Configuration Interaction. Journal of Chemical Theory and Computation, 2020, 16, 5572-5585.	5.3	8
59	Special topic on dynamics of open quantum systems. Journal of Chemical Physics, 2020, 152, 020401.	3.0	8
60	Improving MP2 bandgaps with low-scaling approximations to EOM-CCSD. Journal of Chemical Physics, 2021, 155, 081101.	3.0	8
61	Simplified GW/BSE Approach for Charged and Neutral Excitation Energies of Large Molecules and Nanomaterials. Journal of Chemical Theory and Computation, 2022, 18, 3438-3446.	5.3	7
62	Quantum plasmons and intraband excitons in doped nanoparticles: Insights from quantum chemistry. Journal of Chemical Physics, 2020, 152, 224704.	3.0	5
63	Linear Free Energy Relationships in Electrostatic Catalysis. ACS Catalysis, 2022, 12, 8237-8241.	11.2	5
64	Ab Initio Linear and Pumpâ€“Probe Spectroscopy of Excitons in Molecular Crystals. Journal of Physical Chemistry Letters, 2020, 11, 2241-2246.	4.6	4
65	Polytypism, Anisotropic Transport, and Weyl Nodes in the van der Waals Metal TaFeTe4. Journal of the American Chemical Society, 2021, 143, 109-113.	13.7	4
66	New Directions in the GW/BSE Framework. , 0, , .		0