Diptarka Hait

List of Publications by Year
in descending order

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33 papers	1,942 citations	361413 20 h-index	395702 33 g-index
45 all docs	45 docs citations	45 times ranked	1519 citing authors

#	Article	IF	Citations
1	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
2	How Accurate Is Density Functional Theory at Predicting Dipole Moments? An Assessment Using a New Database of 200 Benchmark Values. Journal of Chemical Theory and Computation, 2018, 14, 1969-1981.	5.3	180
3	Excited State Orbital Optimization via Minimizing the Square of the Gradient: General Approach and Application to Singly and Doubly Excited States via Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 1699-1710.	5.3	106
4	How accurate are static polarizability predictions from density functional theory? An assessment over 132 species at equilibrium geometry. Physical Chemistry Chemical Physics, 2018, 20, 19800-19810.	2.8	94
5	Orbital Optimized Density Functional Theory for Electronic Excited States. Journal of Physical Chemistry Letters, 2021, 12, 4517-4529.	4.6	92
6	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	4.6	90
7	Modern Approaches to Exact Diagonalization and Selected Configuration Interaction with the Adaptive Sampling CI Method. Journal of Chemical Theory and Computation, 2020, 16, 2139-2159.	5.3	90
8	CASSCF with Extremely Large Active Spaces Using the Adaptive Sampling Configuration Interaction Method. Journal of Chemical Theory and Computation, 2020, 16, 2340-2354.	5.3	85
9	Highly Accurate Prediction of Core Spectra of Molecules at Density Functional Theory Cost: Attaining Sub-electronvolt Error from a Restricted Open-Shell Kohnâ€“Sham Approach. Journal of Physical Chemistry Letters, 2020, 11, 775-786.	4.6	82
10	Prediction of Excited-State Energies and Singletâ€“Triplet Gaps of Charge-Transfer States Using a Restricted Open-Shell Kohnâ€“Sham Approach. Journal of Chemical Theory and Computation, 2016, 12, 3353-3359.	5.3	74
11	Delocalization Errors in Density Functional Theory Are Essentially Quadratic in Fractional Occupation Number. Journal of Physical Chemistry Letters, 2018, 9, 6280-6288.	4.6	71
12	Revisiting the Performance of Time-Dependent Density Functional Theory for Electronic Excitations: Assessment of 43 Popular and Recently Developed Functionals from Rungs One to Four. Journal of Chemical Theory and Computation, 2022, 18, 3460-3473.	5.3	61
13	What Levels of Coupled Cluster Theory Are Appropriate for Transition Metal Systems? A Study Using Near-Exact Quantum Chemical Values for 3d Transition Metal Binary Compounds. Journal of Chemical Theory and Computation, 2019, 15, 5370-5385.	5.3	42
14	Revealing the nature of electron correlation in transition metal complexes with symmetry breaking and chemical intuition. Journal of Chemical Physics, 2021, 154, 194109.	3.0	36
15	Chemoenzymatic Platform for Synthesis of Chiral Organofluorines Based on Typeâ€…II Aldolases. Angewandte Chemie - International Edition, 2019, 58, 11841-11845.	13.8	34
16	Accurate prediction of core-level spectra of radicals at density functional theory cost via square gradient minimization and recoupling of mixed configurations. Journal of Chemical Physics, 2020, 153, 134108.	3.0	31
17	Third-Order MÃ¸llerâ€“Plesset Theory Made More Useful? The Role of Density Functional Theory Orbitals. Journal of Chemical Theory and Computation, 2020, 16, 7473-7489.	5.3	27
18	Well-behaved versus ill-behaved density functionals for single bond dissociation: Separating success from disaster functional by functional for stretched H2. Journal of Chemical Physics, 2019, 150, 094115.	3.0	25

#	Article	IF	Citations
19	Relativistic Orbital-Optimized Density Functional Theory for Accurate Core-Level Spectroscopy. Journal of Physical Chemistry Letters, 2022, 13, 3438-3449.	4.6	24
20	Real-Time Evolution for Ultracompact Hamiltonian Eigenstates on Quantum Hardware. PRX Quantum, 2022, 3, .	9.2	24
21	Electronâ€“Nuclear Dynamics Accompanying Proton-Coupled Electron Transfer. Journal of the American Chemical Society, 2021, 143, 3104-3112.	13.7	21
22	Communication: xDH double hybrid functionals can be qualitatively incorrect for non-equilibrium geometries: Dipole moment inversion and barriers to radical-radical association using XYG3 and XYGJ-OS. Journal of Chemical Physics, 2018, 148, 171102.	3.0	20
23	Beyond the Coulsonâ€“Fischer point: characterizing single excitation CI and TDDFT for excited states in single bond dissociations. Physical Chemistry Chemical Physics, 2019, 21, 21761-21775.	2.8	20
24	Generalized single excitation configuration interaction: an investigation into the impact of the inclusion of non-orthogonality on the calculation of core-excited states. Physical Chemistry Chemical Physics, 2020, 22, 8182-8192.	2.8	16
25	Too big, too small, or just right? A benchmark assessment of density functional theory for predicting the spatial extent of the electron density of small chemical systems. Journal of Chemical Physics, 2021, 154, 074109.	3.0	15
26	Chemoenzymatic Platform for Synthesis of Chiral Organofluorines Based on Typeâ€…II Aldolases. Angewandte Chemie, 2019, 131, 11967-11971.	2.0	14
27	Bimetallic Mechanism for Alkyne Cyclotrimerization with a Two-Coordinate Fe Precatalyst. ACS Catalysis, 2020, 10, 7800-7807.	11.2	14
28	Condensed phase electron transfer beyond the Condon approximation. Journal of Chemical Physics, 2016, 145, 214105.	3.0	12
29	Computing x-ray absorption spectra from linear-response particles atop optimized holes. Journal of Chemical Physics, 2022, 156, .	3.0	7
30	Two-Coordinate Iron(I) Complexes on the Edge of Stability: Influence of Dispersion and Steric Effects. Organometallics, 2021, 40, 1758-1764.	2.3	6
31	A hybrid memory kernel approach for condensed phase non-adiabatic dynamics. Journal of Chemical Physics, 2017, 147, 014108.	3.0	5
32	Bimolecular Reaction Dynamics in the Phenylâ€“Silane System: Exploring the Prototype of a Radical Substitution Mechanism. Journal of Physical Chemistry Letters, 2018, 9, 5135-5142.	4.6	3
33	Exploring spin symmetry-breaking effects for static field ionization of atoms: Is there an analog to the Coulsonâ€“Fischer point in bond dissociation?. Journal of Chemical Physics, 2021, 155, 014309.	3.0	1