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	Relativistic Orbital-Optimized Density Functional Theory for Accurate Core-Level Spectroscopy. Journal of Physical Chemistry Letters, 2022, 13, 3438-3449.	4.6	24
2	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
3	Real-Time Evolution for Ultracompact Hamiltonian Eigenstates on Quantum Hardware. PRX Quantum, 2022, 3, .	9.2	24
4	Computing x-ray absorption spectra from linear-response particles atop optimized holes. Journal of Chemical Physics, 2022, 156, .	3.0	7
5	Electronâ€“Nuclear Dynamics Accompanying Proton-Coupled Electron Transfer. Journal of the American Chemical Society, 2021, 143, 3104-3112.	13.7	21
6	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
7	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
8	Orbital Optimized Density Functional Theory for Electronic Excited States. Journal of Physical Chemistry Letters, 2021, 12, 4517-4529.	4.6	92
9	Two-Coordinate Iron(I) Complexes on the Edge of Stability: Influence of Dispersion and Steric Effects. Organometallics, 2021, 40, 1758-1764.	2.3	6
10	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
11	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
12	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
13	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	4.6	90
14	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
15	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
16	Bimetallic Mechanism for Alkyne Cyclotrimerization with a Two-Coordinate Fe Precatalyst. ACS Catalysis, 2020, 10, 7800-7807.	11.2	14
17	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
18	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

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19	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
20	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
21	Chemoenzymatic Platform for Synthesis of Chiral Organofluorines Based on Typeâ€…II Aldolases. Angewandte Chemie, 2019, 131, 11967-11971.	2.0	14
22	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
23	Chemoenzymatic Platform for Synthesis of Chiral Organofluorines Based on Typeâ€…II Aldolases. Angewandte Chemie - International Edition, 2019, 58, 11841-11845.	13.8	34
24	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
25	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
26	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
27	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
28	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
29	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
30	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
31	A hybrid memory kernel approach for condensed phase non-adiabatic dynamics. Journal of Chemical Physics, 2017, 147, 014108.	3.0	5
32	Condensed phase electron transfer beyond the Condon approximation. Journal of Chemical Physics, 2016, 145, 214105.	3.0	12
33	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