Thomas KÃ¶rzdÃ¶rfer

List of Publications by Year
in descending order

41 papers	2,487 citations	218381 26 h-index	276539 41 g-index
43 all docs	43 docs citations	43 times ranked	2720 citing authors

#	Article	IF	Citations
1	Organic Electronic Materials: Recent Advances in the DFT Description of the Ground and Excited States Using Tuned Range-Separated Hybrid Functionals. Accounts of Chemical Research, 2014, 47, 3284-3291.	7.6	324
2	Long-range corrected hybrid functionals for Ï€-conjugated systems: Dependence of the range-separation parameter on conjugation length. Journal of Chemical Physics, 2011, 135, 204107.	1.2	234
3	Benchmark of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>methods for azabenzenes. Physical Review B, 2012, 86, .	1.1	154
4	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules III: A Benchmark of GW Methods. Journal of Chemical Theory and Computation, 2016, 12, 615-626.	2.3	154
5	Ionization Energies, Electron Affinities, and Polarization Energies of Organic Molecular Crystals: Quantitative Estimations from a Polarizable Continuum Model (PCM)-Tuned Range-Separated Density Functional Approach. Journal of Chemical Theory and Computation, 2016, 12, 2906-2916.	2.3	124
6	Communication: Orbital instabilities and triplet states from time-dependent density functional theory and long-range corrected functionals. Journal of Chemical Physics, 2011, 135, 151103.	1.2	117
7	Strategy for finding a reliable starting point for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msub><mml:msub><mml:mi>W</mml:mi> for molecules. Physical Review B, 2012, 86, .	1.1	106
8	When to trust photoelectron spectra from Kohn-Sham eigenvalues: The case of organic semiconductors. Physical Review B, 2009, 79, .	1.1	103
9	On the relationship between bond-length alternation and many-electron self-interaction error. Journal of Chemical Physics, 2012, 137, 124305.	1.2	84
10	Orbital Density Reconstruction for Molecules. Physical Review Letters, 2011, 107, 193002.	2.9	78
11	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules II: Non-Empirically Tuned Long-Range Corrected Hybrid Functionals. Journal of Chemical Theory and Computation, 2016, 12, 605-614.	2.3	78
12	Self-interaction correction and the optimized effective potential. Journal of Chemical Physics, 2008, 129, 014110.	1.2	72
13	Electrical Response of Molecular Systems: The Power of Self-Interaction Corrected Kohn-Sham Theory. Physical Review Letters, 2008, 100, 133004.	2.9	70
14	A Highly K⁺â€Selective Phenylazaâ€[18]crownâ€6â€Lariatâ€Etherâ€Based Fluoroionophore and Its Application in the Sensing of K⁺ Ions with an Optical Sensor Film and in Cells. Chemistry - A European Journal, 2013, 19, 14911-14917.	1.7	66
15	Kohn-Sham Self-Interaction Correction in Real Time. Physical Review Letters, 2012, 108, 146401.	2.9	59
16	Electrical response of molecular chains in density functional theory: Ultranonlocal response from a semilocal functional. Physical Review B, 2008, 77, .	1.1	58
17	Single-particle and quasiparticle interpretation of Kohn-Sham and generalized Kohn-Sham eigenvalues for hybrid functionals. Physical Review B, 2010, 82, .	1.1	58
18	Assessment of the performance of tuned range-separated hybrid density functionals in predicting accurate quasiparticle spectra. Physical Review B, 2012, 86, .	1.1	58

#	Article	IF	Citations
19	Long-Range Corrected DFT Meets GW: Vibrationally Resolved Photoelectron Spectra from First Principles. Journal of Chemical Theory and Computation, 2015, 11, 5391-5400.	2.3	46
20	Sequence dependence of electron-induced DNA strand breakage revealed by DNA nanoarrays. Scientific Reports, 2014, 4, 7391.	1.6	45
21	Collectively Induced Quantum-Confined Stark Effect in Monolayers of Molecules Consisting of Polar Repeating Units. Journal of the American Chemical Society, 2011, 133, 18634-18645.	6.6	33
22	Accurate description of torsion potentials in conjugated polymers using density functionals with reduced self-interaction error. Journal of Chemical Physics, 2014, 140, 054310.	1.2	32
23	On the relation between orbital-localization and self-interaction errors in the density functional theory treatment of organic semiconductors. Journal of Chemical Physics, 2011, 134, 094111.	1.2	30
24	Size Effects in the Interface Level Alignment of Dye-Sensitized TiO₂ Clusters. Journal of Physical Chemistry Letters, 2014, 5, 2395-2401.	2.1	28
25	Synthesis of donor-substituted meso-phenyl and meso-ethynylphenyl BODIPYs with broad absorption. New Journal of Chemistry, 2013, 37, 1417.	1.4	27
26	Toward a Robust Quantum-Chemical Description of Organic Mixed-Valence Systems. Journal of Physical Chemistry C, 2014, 118, 3925-3934.	1.5	23
27	Calculating Optical Absorption Spectra of Thin Polycrystalline Organic Films: Structural Disorder and Site-Dependent van der Waals Interaction. Journal of Physical Chemistry C, 2015, 119, 5747-5751.	1.5	22
28	Energy transfer and FÃ¶rsterâ€™s dipole coupling approximation investigated in a real-time Kohn-Sham scheme. Physical Review A, 2010, 82, .	1.0	20
29	Computational high throughput screening of inorganic cation based halide perovskites for perovskite only tandem solar cells. Materials Research Express, 2020, 7, 055502.	0.8	19
30	Efficient Palladium(II) Precatalysts Bearing 4,5â€Dicyanoimidazolâ€2â€ylidene for the Mizorokiâ€“Heck Reaction. European Journal of Inorganic Chemistry, 2014, 2014, 2952-2960.	1.0	18
31	Size-Dependence of Nonempirically Tuned DFT Starting Points for G₀W₀ Applied to Ï€-Conjugated Molecular Chains. Journal of Chemical Theory and Computation, 2017, 13, 4962-4971.	2.3	16
32	Metal Sulfide Nanoparticle Synthesis with Ionic Liquids â€“ State of the Art and Future Perspectives. ChemistryOpen, 2021, 10, 272-295.	0.9	16
33	Fluorescence quenching in an organic donor-acceptor dyad: A first principles study. Journal of Chemical Physics, 2009, 131, 034310.	1.2	15
34	Computational screening of methylammonium based halide perovskites with bandgaps suitable for perovskite-perovskite tandem solar cells. Journal of Chemical Physics, 2018, 149, 214701.	1.2	14
35	Accurate Valence Ionization Energies from Kohnâ€“Sham Eigenvalues with the Help of Potential Adjustors. Journal of Chemical Theory and Computation, 2017, 13, 4726-4740.	2.3	11
36	How Bond Length Alternation and Thermal Disorder Affect the Optical Excitation Energies of Ï€-Conjugated Chains: A Combined Density Functional Theory and Molecular Dynamics Study. Journal of Chemical Theory and Computation, 2016, 12, 1872-1882.	2.3	10

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37	Vibrationally resolved photoelectron spectra of lower diamondoids: A time-dependent approach. Journal of Chemical Physics, 2018, 148, 044310.	1.2	9
38	Alkylpyridinium Tetrahalidometallate Ionic Liquids and Ionic Liquid Crystals: Insights into the Origin of Their Phase Behavior. European Journal of Inorganic Chemistry, 2017, 2017, 5640-5649.	1.0	7
39	The 1,6,7,12â€Tetraazaperylene Bridging Ligand as an Electron Reservoir and Its Disulfonato Derivative as Redox Mediator in an Enzymeâ€“Electrode Process. Chemistry - A European Journal, 2017, 23, 15583-15587.	1.7	4
40	Reply to â€œComment on â€˜Calculating Optical Absorption Spectra of Thin Polycrystalline Organic Films: Structural Disorder and Site-Dependent van der Waals Interactionâ€™â€• Journal of Physical Chemistry C, 2015, 119, 18818-18820.	1.5	3
41	DFT 101 and Applications to Ï€-Conjugated Systems. Materials and Energy, 2016, , 19-52.	2.5	0