

# Carlo Adamo

## List of Publications by Year in descending order

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449  
papers

43,384  
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5876

81  
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2439

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469  
docs citations

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times ranked

30612  
citing authors

#	ARTICLE	IF	CITATIONS
1	Toward reliable density functional methods without adjustable parameters: The PBE0 model. <i>Journal of Chemical Physics</i> , 1999, 110, 6158-6170.	1.2	14,178
2	Exchange functionals with improved long-range behavior and adiabatic connection methods without adjustable parameters: The mPW and mPW1PW models. <i>Journal of Chemical Physics</i> , 1998, 108, 664-675.	1.2	3,068
3	The calculations of excited-state properties with Time-Dependent Density Functional Theory. <i>Chemical Society Reviews</i> , 2013, 42, 845-856.	18.7	1,424
4	Extensive TD-DFT Benchmark: Singlet-Excited States of Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2420-2435.	2.3	942
5	A Qualitative Index of Spatial Extent in Charge-Transfer Excitations. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2498-2506.	2.3	858
6	TD-DFT Performance for the Visible Absorption Spectra of Organic Dyes: Conventional versus Long-Range Hybrids. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 123-135.	2.3	766
7	Toward reliable adiabatic connection models free from adjustable parameters. <i>Chemical Physics Letters</i> , 1997, 274, 242-250.	1.2	706
8	Accurate excitation energies from time-dependent density functional theory: Assessing the PBE0 model. <i>Journal of Chemical Physics</i> , 1999, 111, 2889-2899.	1.2	661
9	Accurate Simulation of Optical Properties in Dyes. <i>Accounts of Chemical Research</i> , 2009, 42, 326-334.	7.6	435
10	TD-DFT Assessment of Functionals for Optical $\pi \rightarrow \pi^*$ Transitions in Solvated Dyes. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2359-2372.	2.3	403
11	On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2071-2085.	2.3	383
12	Mechanism of the Palladium-Catalyzed Homocoupling of Arylboronic Acids: Key Involvement of a Palladium Peroxo Complex. <i>Journal of the American Chemical Society</i> , 2006, 128, 6829-6836.	6.6	345
13	On the Metric of Charge Transfer Molecular Excitations: A Simple Chemical Descriptor. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3118-3126.	2.3	335
14	Density functional theory analysis of the structural and electronic properties of TiO <sub>2</sub> rutile and anatase polytypes: Performances of different exchange-correlation functionals. <i>Journal of Chemical Physics</i> , 2007, 126, 154703.	1.2	307
15	Excited-state calculations with TD-DFT: from benchmarks to simulations in complex environments. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 16987.	1.3	301
16	Dye chemistry with time-dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14334-14356.	1.3	294
17	Assessment of the efficiency of long-range corrected functionals for some properties of large compounds. <i>Journal of Chemical Physics</i> , 2007, 126, 144105.	1.2	290
18	What is the "best" atomic charge model to describe through-space charge-transfer excitations?. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 5383.	1.3	290

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19	Toward chemical accuracy in the computation of NMR shieldings: the PBE0 model. <i>Chemical Physics Letters</i> , 1998, 298, 113-119.	1.2	266
20	Choosing a Functional for Computing Absorption and Fluorescence Band Shapes with TD-DFT. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2749-2760.	2.3	243
21	Seeking for parameter-free double-hybrid functionals: The PBE0-DH model. <i>Journal of Chemical Physics</i> , 2011, 135, 024106.	1.2	226
22	Through-Space Charge Transfer in Rod-Like Molecules: Lessons from Theory. <i>Journal of Physical Chemistry C</i> , 2012, 116, 11946-11955.	1.5	222
23	Proton transfer in the ground and lowest excited states of malonaldehyde: A comparative density functional and post-Hartree-Fock study. <i>Journal of Chemical Physics</i> , 1996, 105, 11007-11019.	1.2	215
24	Photoinduced Intramolecular Electron Transfer in Ruthenium and Osmium Polyads: Insights from Theory. <i>Journal of the American Chemical Society</i> , 2004, 126, 10763-10777.	6.6	210
25	A TDDFT study of the electronic spectrum of s-tetrazine in the gas-phase and in aqueous solution. <i>Chemical Physics Letters</i> , 2000, 330, 152-160.	1.2	205
26	Structural and Electronic Properties of Selected Rutile and Anatase TiO <sub>2</sub> Surfaces: An ab Initio Investigation. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 341-352.	2.3	204
27	Assessment of Functionals for TD-DFT Calculations of Singlet-Triplet Transitions. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1532-1537.	2.3	194
28	First-Principles Modeling of Dye-Sensitized Solar Cells: Challenges and Perspectives. <i>Accounts of Chemical Research</i> , 2012, 45, 1268-1277.	7.6	194
29	Predicting proton transfer barriers with density functional methods. <i>Chemical Physics Letters</i> , 1999, 306, 83-87.	1.2	178
30	A Theoretical Investigation of the Ground and Excited States of Selected Ru and Os Polypyridyl Molecular Dyes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11354-11360.	1.1	174
31	On the Calculation and Modeling of Magnetic Exchange Interactions in Weakly Bonded Systems: The Case of the Ferromagnetic Copper(II) $\mu_2$ -Azido Bridged Complexes. <i>Inorganic Chemistry</i> , 1999, 38, 1996-2004.	1.9	173
32	Conformational behavior of gaseous glycine by a density functional approach. <i>Journal of Chemical Physics</i> , 1995, 102, 364-370.	1.2	171
33	An accurate density functional method for the study of magnetic properties: the PBE0 model. <i>Computational and Theoretical Chemistry</i> , 1999, 493, 145-157.	1.5	168
34	Benchmarking Density Functionals on Structural Parameters of Small-/Medium-Sized Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 459-465.	2.3	165
35	A TD-DFT investigation of ground and excited state properties in indoline dyes used for dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 11276.	1.3	161
36	First hyperpolarizability of polymethineimine with long-range corrected functionals. <i>Journal of Chemical Physics</i> , 2007, 126, 191108.	1.2	158

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37	Communication: Double-hybrid functionals from adiabatic-connection: The QIDH model. <i>Journal of Chemical Physics</i> , 2014, 141, 031101.	1.2	154
38	Inexpensive and accurate predictions of optical excitations in transition-metal complexes: the TDDFT/PBE0 route. <i>Theoretical Chemistry Accounts</i> , 2000, 105, 169-172.	0.5	141
39	Validation of self-consistent hybrid density functionals for the study of structural and electronic characteristics of organic $\dot{\text{I}}$ radicals. <i>Journal of Chemical Physics</i> , 1995, 102, 384-393.	1.2	138
40	Physically motivated density functionals with improved performances: The modified Perdew-Burke-Ernzerhof model. <i>Journal of Chemical Physics</i> , 2002, 116, 5933-5940.	1.2	138
41	Performance of an Optimally Tuned Range-Separated Hybrid Functional for $\text{O}=\text{O}$ Electronic Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1677-1685.	2.3	135
42	Assessment of the B97 family for excited-state calculations. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 127-136.	0.5	132
43	Bond Length Alternation of Conjugated Oligomers: Wave Function and DFT Benchmarks. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 369-376.	2.3	131
44	Planar vs. twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 8016.	1.3	126
45	First Principles Modeling of Eosin-Loaded ZnO Films: A Step toward the Understanding of Dye-Sensitized Solar Cell Performances. <i>Journal of the American Chemical Society</i> , 2009, 131, 14290-14298.	6.6	124
46	Verdict: Time-Dependent Density Functional Theory is Not Guilty of Large Errors for Cyanines. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1255-1259.	2.3	122
47	Assessment of long-range corrected functionals performance for $\pi\pi^*$ transitions in organic dyes. <i>Journal of Chemical Physics</i> , 2007, 127, 094102.	1.2	119
48	Accurate Evaluation of Valence and Low-Lying Rydberg States with Standard Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5549-5556.	1.1	119
49	Contribution to the Mechanism of Copper-Catalyzed $\text{C}=\text{N}$ and $\text{C}=\text{O}$ Bond Formation. <i>Organometallics</i> , 2012, 31, 7694-7707.	1.1	119
50	Exploring excited states using Time Dependent Density Functional Theory and density-based indexes. <i>Coordination Chemistry Reviews</i> , 2015, 304-305, 166-178.	9.5	118
51	Accurate excitation energies from time-dependent density functional theory: assessing the PBE0 model for organic free radicals. <i>Chemical Physics Letters</i> , 1999, 314, 152-157.	1.2	116
52	A General Guidebook for the Theoretical Prediction of Physicochemical Properties of Chemicals for Regulatory Purposes. <i>Chemical Reviews</i> , 2015, 115, 13093-13164.	23.0	116
53	Time-dependent density functional theory investigation of the absorption, fluorescence, and phosphorescence spectra of solvated coumarins. <i>Journal of Chemical Physics</i> , 2006, 125, 164324.	1.2	115
54	Communication: One third: A new recipe for the PBE0 paradigm. <i>Journal of Chemical Physics</i> , 2013, 138, 021104.	1.2	115

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55	The meta-GGA functional: Thermochemistry with a kinetic energy density dependent exchange-correlation functional. <i>Journal of Chemical Physics</i> , 2000, 112, 2643-2649.	1.2	114
56	TD-DFT Vibronic Couplings in Anthraquinones: From Basis Set and Functional Benchmarks to Applications for Industrial Dyes. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1882-1892.	2.3	113
57	Electronic Excitations in Solution: The Interplay between State Specific Approaches and a Time-Dependent Density Functional Theory Description. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5782-5790.	2.3	112
58	Surface-dependent oxidation of H <sub>2</sub> on CeO <sub>2</sub> surfaces. <i>Journal of Catalysis</i> , 2013, 297, 193-201.	3.1	109
59	Phototriggered Linkage Isomerization in Ruthenium <sup>II</sup> -Dimethylsulfoxide Complexes: Insights from Theory. <i>Journal of Physical Chemistry A</i> , 2003, 107, 11182-11190.	1.1	108
60	Spectroscopic Properties of Porphyrin-Like Photosensitizers: Insights from Theory. <i>Journal of Physical Chemistry B</i> , 2006, 110, 2398-2404.	1.2	106
61	Modeling Dye-Sensitized Solar Cells: From Theory to Experiment. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1044-1050.	2.1	104
62	Nonempirical Double-Hybrid Functionals: An Effective Tool for Chemists. <i>Accounts of Chemical Research</i> , 2016, 49, 1503-1513.	7.6	103
63	Performance of the 'parameter free' PBE0 functional for the modeling of molecular properties of heavy metals. <i>Chemical Physics Letters</i> , 2000, 325, 99-105.	1.2	100
64	Orthorhombic $\text{BiFeO}_3$ . <i>Physical Review Letters</i> , 2012, 109, 247606.	2.9	100
65	Double-hybrid density functionals: merging wavefunction and density approaches to get the best of both worlds. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14581.	1.3	100
66	Proton transfer in model hydrogen-bonded systems by a density functional approach. <i>Chemical Physics Letters</i> , 1994, 231, 295-300.	1.2	99
67	A hybrid density functional study of the first $\pi$ transition in metal monocarbonyls. <i>Journal of Chemical Physics</i> , 1995, 103, 10605-10613.	1.2	99
68	Comment on "About the calculation of exchange coupling constants using density-functional theory: The role of the self-interaction error". <i>J. Chem. Phys.</i> 123, 164110 (2005). <i>Journal of Chemical Physics</i> , 2006, 124, 107101.	1.2	99
69	Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. <i>Journal of Chemical Physics</i> , 2012, 136, 174103.	1.2	99
70	Extensive TD-DFT investigation of the first electronic transition in substituted azobenzenes. <i>Chemical Physics Letters</i> , 2008, 465, 226-229.	1.2	96
71	Is the Tamm-Dancoff Approximation Reliable for the Calculation of Absorption and Fluorescence Band Shapes?. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4517-4525.	2.3	95
72	Density Functional Study of Intrinsic and Environmental Effects in the Tautomeric Equilibrium of 2-Pyridone. <i>The Journal of Physical Chemistry</i> , 1995, 99, 15062-15068.	2.9	94

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73	A Theoretical Study of Bonding in Lanthanide Trihalides by Density Functional Methods. <i>Journal of Physical Chemistry A</i> , 1998, 102, 6812-6820.	1.1	94
74	Communication: Rationale for a new class of double-hybrid approximations in density-functional theory. <i>Journal of Chemical Physics</i> , 2011, 135, 101102.	1.2	93
75	Implementation and validation of the Lacks-Gordon exchange functional in conventional density functional and adiabatic connection methods. <i>Journal of Computational Chemistry</i> , 1998, 19, 418-429.	1.5	91
76	Comparative studies of quasi-relativistic density functional methods for the description of lanthanide and actinide complexes. <i>Journal of Computational Chemistry</i> , 2003, 24, 850-858.	1.5	89
77	Localized Excited Charge Carriers Generate Ultrafast Inhomogeneous Strain in the Multiferroic $\text{BiFeO}_3$ . <i>Physical Review Letters</i> , 2014, 112, 097602.	2.9	89
78	Accurate static polarizabilities by density functional theory: assessment of the PBE0 model. <i>Chemical Physics Letters</i> , 1999, 307, 265-271.	1.2	86
79	DFT and Proton Transfer Reactions: A Benchmark Study on Structure and Kinetics. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3082-3088.	2.3	85
80	Validation and assessment of an accurate approach to the correlation problem in density functional theory: The Kriger-Chen-Savin model. <i>Journal of Chemical Physics</i> , 2002, 117, 10465-10473.	1.2	83
81	Theoretical study of direct and water-assisted isomerization of formaldehyde radical cation. A comparison between density functional and post-Hartree-Fock approaches. <i>Chemical Physics Letters</i> , 1994, 224, 432-438.	1.2	82
82	Impact of Vibronic Couplings on Perceived Colors: Two Anthraquinones as a Working Example. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 468-471.	2.1	82
83	Predictions of Optical Excitations in Transition-Metal Complexes with Time Dependent-Density Functional Theory: Influence of Basis Sets. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 953-962.	2.3	80
84	Toward a Clear-Cut Vision on the Origin of 2,6-Di(1,2,4-triazin-3-yl)pyridine Selectivity for Trivalent Actinides: Insights from Theory. <i>Inorganic Chemistry</i> , 2006, 45, 8517-8522.	1.9	77
85	Assessment of Several Hybrid DFT Functionals for the Evaluation of Bond Length Alternation of Increasingly Long Oligomers. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5952-5959.	1.1	77
86	Absorption Spectra of First-Row Transition Metal Complexes of Bacteriochlorins: A Theoretical Analysis. <i>Journal of Physical Chemistry B</i> , 2005, 109, 12214-12221.	1.2	76
87	A Comprehensive Theoretical View of the Bonding in Actinide Molecular Complexes. <i>Journal of the American Chemical Society</i> , 2006, 128, 2190-2191.	6.6	76
88	On the TD-DFT Accuracy in Determining Single and Double Bonds in Excited-State Structures of Organic Molecules. <i>Journal of Physical Chemistry A</i> , 2010, 114, 13402-13410.	1.1	76
89	Ab Initio Molecular Dynamics Study of a Highly Concentrated LiCl Aqueous Solution. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1040-1048.	2.3	74
90	Accuracy of TD-DFT Geometries: A Fresh Look. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3715-3727.	2.3	74

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91	Oxidation mechanism of diethyl ether: a complex process for a simple molecule. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14636.	1.3	73
92	Theoretical Unraveling of Selective 1-Butene Oligomerization Catalyzed by Iron <sup>II</sup> Bis(arylimino)pyridine. <i>Organometallics</i> , 2009, 28, 5358-5367.	1.1	72
93	Insights into Working Principles of Ruthenium Polypyridyl Dye-Sensitized Solar Cells from First Principles Modeling. <i>Journal of Physical Chemistry C</i> , 2011, 115, 4297-4306.	1.5	71
94	Absorption and emission spectra in gas-phase and solution using TD-DFT: Formaldehyde and benzene as case studies. <i>Chemical Physics Letters</i> , 2006, 421, 272-276.	1.2	70
95	Evaluating push-pull dye efficiency using TD-DFT and charge transfer indices. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 20210.	1.3	68
96	Functionalized Graphene as an Electron-Cascade Acceptor for Air-Processed Organic Ternary Solar Cells. <i>Advanced Functional Materials</i> , 2015, 25, 3870-3880.	7.8	67
97	Ionic versus covalent character in lanthanide complexes. A hybrid density functional study. <i>Chemical Physics Letters</i> , 1997, 268, 61-68.	1.2	66
98	First-row transition-metal hydrides: A challenging playground for new theoretical approaches. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 443-451.	1.0	65
99	Theoretical Study of the Addition of Hydrogen Cyanide to Methanimine in the Gas Phase and in Aqueous Solution. <i>Journal of the American Chemical Society</i> , 2000, 122, 324-330.	6.6	65
100	Complete structural and magnetic characterization of biological radicals in solution by an integrated quantum mechanical approach: Glycyl radical as a case study. <i>Journal of Chemical Physics</i> , 2004, 121, 6710-6718.	1.2	65
101	Designing Multifunctional Expanded Pyridiniums: Properties of Branched and Fused Head-to-Tail Bipyridiniums. <i>Journal of the American Chemical Society</i> , 2010, 132, 16700-16713.	6.6	65
102	The geometries, absorption and fluorescence wavelengths of solvated fluorescent coumarins: A CIS and TD-DFT comparative study. <i>Chemical Physics Letters</i> , 2007, 438, 208-212.	1.2	63
103	Effective electron displacements: A tool for time-dependent density functional theory computational spectroscopy. <i>Journal of Chemical Physics</i> , 2014, 140, 104101.	1.2	63
104	A comprehensive DFT investigation of bulk and low-index surfaces of ZrO <sub>2</sub> polymorphs. <i>Journal of Computational Chemistry</i> , 2015, 36, 9-21.	1.5	61
105	Range-separated hybrid density functionals made simple. <i>Journal of Chemical Physics</i> , 2019, 150, 201102.	1.2	60
106	Theoretical Insights on O <sub>2</sub> and CO Adsorption on Neutral and Positively Charged Gold Clusters. <i>Journal of Physical Chemistry B</i> , 2006, 110, 12240-12248.	1.2	58
107	Absorption and emission spectra of 1,8-naphthalimide fluorophores: A PCM-TD-DFT investigation. <i>Chemical Physics</i> , 2010, 372, 61-66.	0.9	58
108	Structure and magnetic properties of benzyl, anilino, and phenoxy radicals by density functional computations. <i>Journal of Chemical Physics</i> , 1998, 109, 10244-10254.	1.2	57

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109	Spectral properties of self-assembled squaraine tetralactam: a theoretical assessment. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 1258.	1.3	57
110	Excited-State Geometries of Heteroaromatic Compounds: A Comparative TD-DFT and SAC-CI Study. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2368-2379.	2.3	57
111	The nature of vertical excited states of dyes containing metals for DSSC applications: insights from TD-DFT and density based indexes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14435.	1.3	57
112	Theoretical Exploration of Type I/Type II Dual Photoreactivity of Promising Ru(II) Dyads for PDT Approach. <i>Inorganic Chemistry</i> , 2016, 55, 11185-11192.	1.9	57
113	Theoretical Investigation on the Role of the Central Carbon Atom and Close Protein Environment on the Nitrogen Reduction in Mo Nitrogenase. <i>ACS Catalysis</i> , 2016, 6, 1567-1577.	5.5	57
114	Density functional approach to the structures and EPR parameters of open shell systems. The case of fluorovinyl radicals. <i>Chemical Physics Letters</i> , 1993, 212, 5-11.	1.2	56
115	On the TD-DFT UV/vis spectra accuracy: the azoalkanes. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 405-410.	0.5	56
116	A new parameter-free correlation functional based on an average atomic reduced density gradient analysis. <i>Journal of Chemical Physics</i> , 2008, 128, 034101.	1.2	56
117	From Classical Density Functionals to Adiabatic Connection Methods. The State of the Art.. <i>Advances in Quantum Chemistry</i> , 2000, 36, 45-75.	0.4	53
118	Understanding Aggregation-Induced Emission in Molecular Crystals: Insights from Theory. <i>Journal of Physical Chemistry C</i> , 2017, 121, 5747-5752.	1.5	52
119	Assessment of recently developed density functional approaches for the evaluation of the bond length alternation in polyacetylene. <i>Chemical Physics Letters</i> , 2005, 405, 376-381.	1.2	51
120	Exploring the Metric of Excited State Proton Transfer Reactions. <i>Journal of Physical Chemistry B</i> , 2013, 117, 16165-16173.	1.2	51
121	Performance of the $\bar{I}_n$ -dependent functionals in predicting the magnetic coupling of ionic antiferromagnetic insulators. <i>Journal of Chemical Physics</i> , 2004, 120, 3811-3816.	1.2	50
122	Self-interaction error in density functional theory: a mean-field correction for molecules and large systems. <i>Chemical Physics</i> , 2005, 309, 67-76.	0.9	50
123	Morphological and charge transport properties of amorphous and crystalline P3HT and PBTTT: insights from theory. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 18742-18750.	1.3	50
124	Transport properties in manganite thin films. <i>Physical Review B</i> , 2005, 71, .	1.1	49
125	A mean-field self-interaction correction in density functional theory: implementation and validation for molecules. <i>Chemical Physics Letters</i> , 2003, 380, 12-20.	1.2	48
126	Solvent effects on an SN2 reaction profile. <i>Chemical Physics Letters</i> , 1998, 297, 1-7.	1.2	46



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127	Density Functional Study of Diborane, Dialane, and Digallane. <i>The Journal of Physical Chemistry</i> , 1994, 98, 13185-13188.	2.9	45
128	Theoretical Study of the Decomposition Reactions in Substituted Nitrobenzenes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4054-4059.	1.1	45
129	Range-Separated Double-Hybrid Functional from Nonempirical Constraints. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4052-4062.	2.3	45
130	Comparison of conventional and hybrid density functional approaches. Cationic hydrides of first-row transition metals as a case study. <i>Chemical Physics Letters</i> , 1996, 249, 290-296.	1.2	44
131	Catalytic and bulk solvent effects on proton transfer: Formamide as a case study. <i>Journal of Computational Chemistry</i> , 1997, 18, 1993-2000.	1.5	44
132	Intramolecular Spin Alignment in Photomagnetic Molecular Devices: A Theoretical Study. <i>Chemistry - A European Journal</i> , 2007, 13, 5360-5377.	1.7	44
133	Computational Protocol for Modeling Thermochromic Molecular Crystals: Salicylidene Aniline As a Case Study. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5577-5585.	2.3	44
134	Electronic Band Shapes Calculated with Optimally Tuned Range-Separated Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4599-4608.	2.3	44
135	Non-radiative decay paths in rhodamines: new theoretical insights. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 20681-20688.	1.3	44
136	Theoretical Investigation of Hole Transporter Materials for Energy Devices. <i>Journal of Physical Chemistry C</i> , 2015, 119, 23890-23898.	1.5	44
137	Systematic Improvement of Density Functionals through Parameter-Free Hybridization Schemes. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 3540-3545.	2.1	44
138	Charge transfer excitations in TDDFT: A ghost-hunter index. <i>Journal of Computational Chemistry</i> , 2017, 38, 2151-2156.	1.5	44
139	Photoinduced Processes within Compact Dyads Based on Triphenylpyridinium-Functionalized Bipyridyl Complexes of Ruthenium(II). <i>Chemistry - A European Journal</i> , 2005, 11, 3711-3727.	1.7	43
140	Fluorescence of 1,8-naphthalimide: A PCM-TD-DFT investigation. <i>Chemical Physics Letters</i> , 2007, 448, 3-6.	1.2	43
141	Modeling ZnO phases using a periodic approach: From bulk to surface and beyond. <i>Journal of Chemical Physics</i> , 2009, 131, 044708.	1.2	43
142	A Theoretical Study of the Decomposition Mechanisms in Substituted o-Nitrotoluenes. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13621-13627.	1.1	43
143	The ammonium nitrate and its mechanism of decomposition in the gas phase: a theoretical study and a DFT benchmark. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10849.	1.3	43
144	Structure and ESR features of glycine radical in its zwitterionic form. <i>Chemical Physics Letters</i> , 1995, 242, 351-354.	1.2	42

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145	Bi-isonicotinic Acid on Anatase (101): Insights from Theory. <i>Journal of Physical Chemistry C</i> , 2007, 111, 15034-15042.	1.5	42
146	Phosphorescent Binuclear Iridium Complexes Based on Terpyridine-Carboxylate: An Experimental and Theoretical Study. <i>Inorganic Chemistry</i> , 2011, 50, 8197-8206.	1.9	42
147	Influence of the Formation of the Halogen Bond ArX-N on the Mechanism of Diketonate Ligated Copper-Catalyzed Amination of Aromatic Halides. <i>Organometallics</i> , 2012, 31, 914-920.	1.1	42
148	Double hybrids and time-dependent density functional theory: An implementation and benchmark on charge transfer excited states. <i>Journal of Computational Chemistry</i> , 2020, 41, 1242-1251.	1.5	42
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