Carlo Adamo

List of Publications by Year
in descending order

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449 papers	43,384 citations	5896 81 h-index	2448 197 g-index
469 all docs	469 docs citations	469 times ranked	30612 citing authors

#	Article	IF	Citations
1	Toward reliable density functional methods without adjustable parameters: The PBE0 model. Journal of Chemical Physics, 1999, 110, 6158-6170.	3.0	14,178
2	Exchange functionals with improved long-range behavior and adiabatic connection methods without adjustable parameters: The mPW and mPW1PW models. Journal of Chemical Physics, 1998, 108, 664-675.	3.0	3,068
3	The calculations of excited-state properties with Time-Dependent Density Functional Theory. Chemical Society Reviews, 2013, 42, 845-856.	38.1	1,424
4	Extensive TD-DFT Benchmark: Singlet-Excited States of Organic Molecules. Journal of Chemical Theory and Computation, 2009, 5, 2420-2435.	5.3	942
5	A Qualitative Index of Spatial Extent in Charge-Transfer Excitations. Journal of Chemical Theory and Computation, 2011, 7, 2498-2506.	5.3	858
6	TD-DFT Performance for the Visible Absorption Spectra of Organic Dyes:â€‰ Conventional versus Long-Range Hybrids. Journal of Chemical Theory and Computation, 2008, 4, 123-135.	5.3	766
7	Toward reliable adiabatic connection models free from adjustable parameters. Chemical Physics Letters, 1997, 274, 242-250.	2.6	706
8	Accurate excitation energies from time-dependent density functional theory: Assessing the PBE0 model. Journal of Chemical Physics, 1999, 111, 2889-2899.	3.0	661
9	Accurate Simulation of Optical Properties in Dyes. Accounts of Chemical Research, 2009, 42, 326-334.	15.6	435
10	TD-DFT Assessment of Functionals for Optical 0â€“0 Transitions in Solvated Dyes. Journal of Chemical Theory and Computation, 2012, 8, 2359-2372.	5.3	403
11	On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies. Journal of Chemical Theory and Computation, 2010, 6, 2071-2085.	5.3	383
12	Mechanism of the Palladium-Catalyzed Homocoupling of Arylboronic Acids:â€‰ Key Involvement of a Palladium Peroxo Complex. Journal of the American Chemical Society, 2006, 128, 6829-6836.	13.7	345
13	On the Metric of Charge Transfer Molecular Excitations: A Simple Chemical Descriptor. Journal of Chemical Theory and Computation, 2013, 9, 3118-3126.	5.3	335
14	Density functional theory analysis of the structural and electronic properties of TiO2 rutile and anatase polytypes: Performances of different exchange-correlation functionals. Journal of Chemical Physics, 2007, 126, 154703.	3.0	307
15	Excited-state calculations with TD-DFT: from benchmarks to simulations in complex environments. Physical Chemistry Chemical Physics, 2011, 13, 16987.	2.8	301
16	Dye chemistry with time-dependent density functional theory. Physical Chemistry Chemical Physics, 2014, 16, 14334-14356.	2.8	294
17	Assessment of the efficiency of long-range corrected functionals for some properties of large compounds. Journal of Chemical Physics, 2007, 126, 144105.	3.0	290
18	What is the â€œbestâ€•atomic charge model to describe through-space charge-transfer excitations?. Physical Chemistry Chemical Physics, 2012, 14, 5383.	2.8	290

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19	Toward chemical accuracy in the computation of NMR shieldings: the PBE0 model. Chemical Physics Letters, 1998, 298, 113-119.	2.6	266
20	Choosing a Functional for Computing Absorption and Fluorescence Band Shapes with TD-DFT. Journal of Chemical Theory and Computation, 2013, 9, 2749-2760.	5.3	243
21	Seeking for parameter-free double-hybrid functionals: The PBE0-DH model. Journal of Chemical Physics, 2011, 135, 024106.	3.0	226
22	Through-Space Charge Transfer in Rod-Like Molecules: Lessons from Theory. Journal of Physical Chemistry C, 2012, 116, 11946-11955.	3.1	222
23	Proton transfer in the ground and lowest excited states of malonaldehyde: A comparative density functional and postâ€Hartreeâ€“Fock study. Journal of Chemical Physics, 1996, 105, 11007-11019.	3.0	215
24	Photoinduced Intramolecular Electron Transfer in Ruthenium and Osmium Polyads:Â Insights from Theory. Journal of the American Chemical Society, 2004, 126, 10763-10777.	13.7	210
25	A TDDFT study of the electronic spectrum of s-tetrazine in the gas-phase and in aqueous solution. Chemical Physics Letters, 2000, 330, 152-160.	2.6	205
26	Structural and Electronic Properties of Selected Rutile and Anatase TiO₂Surfaces:â€‰ An ab Initio Investigation. Journal of Chemical Theory and Computation, 2008, 4, 341-352.	5.3	204
27	Assessment of Functionals for TD-DFT Calculations of Singletâ^'Triplet Transitions. Journal of Chemical Theory and Computation, 2010, 6, 1532-1537.	5.3	194
28	First-Principles Modeling of Dye-Sensitized Solar Cells: Challenges and Perspectives. Accounts of Chemical Research, 2012, 45, 1268-1277.	15.6	194
29	Predicting proton transfer barriers with density functional methods. Chemical Physics Letters, 1999, 306, 83-87.	2.6	178
30	A Theoretical Investigation of the Ground and Excited States of Selected Ru and Os Polypyridyl Molecular Dyes. Journal of Physical Chemistry A, 2002, 106, 11354-11360.	2.5	174
31	On the Calculation and Modeling of Magnetic Exchange Interactions in Weakly Bonded Systems:Â The Case of the Ferromagnetic Copper(II) Î¼2-Azido Bridged Complexes. Inorganic Chemistry, 1999, 38, 1996-2004.	4.0	173
32	Conformational behavior of gaseous glycine by a density functional approach. Journal of Chemical Physics, 1995, 102, 364-370.	3.0	171
33	An accurate density functional method for the study of magnetic properties: the PBE0 model. Computational and Theoretical Chemistry, 1999, 493, 145-157.	1.5	168
34	Benchmarking Density Functionals on Structural Parameters of Small-/Medium-Sized Organic Molecules. Journal of Chemical Theory and Computation, 2016, 12, 459-465.	5.3	165
35	A TD-DFT investigation of ground and excited state properties in indoline dyes used for dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2009, 11, 11276.	2.8	161
36	First hyperpolarizability of polymethineimine with long-range corrected functionals. Journal of Chemical Physics, 2007, 126, 191108.	3.0	158

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37	Communication: Double-hybrid functionals from adiabatic-connection: The QIDH model. Journal of Chemical Physics, 2014, 141, 031101.	3.0	154
38	Inexpensive and accurate predictions of optical excitations in transition-metal complexes: the TDDFT/PBE0 route. Theoretical Chemistry Accounts, 2000, 105, 169-172.	1.4	141
39	Validation of selfâ€consistent hybrid density functionals for the study of structural and electronic characteristics of organic Ï€ radicals. Journal of Chemical Physics, 1995, 102, 384-393.	3.0	138
40	Physically motivated density functionals with improved performances: The modified Perdewâ€“Burkeâ€“Ernzerhof model. Journal of Chemical Physics, 2002, 116, 5933-5940.	3.0	138
41	Performance of an Optimally Tuned Range-Separated Hybrid Functional for 0â€“0 Electronic Excitation Energies. Journal of Chemical Theory and Computation, 2014, 10, 1677-1685.	5.3	135
42	Assessment of the Ï‰B97 family for excited-state calculations. Theoretical Chemistry Accounts, 2011, 128, 127-136.	1.4	132
43	Bond Length Alternation of Conjugated Oligomers: Wave Function and DFT Benchmarks. Journal of Chemical Theory and Computation, 2011, 7, 369-376.	5.3	131
44	Planar vs. twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory. Physical Chemistry Chemical Physics, 2010, 12, 8016.	2.8	126
45	First Principles Modeling of Eosin-Loaded ZnO Films: A Step toward the Understanding of Dye-Sensitized Solar Cell Performances. Journal of the American Chemical Society, 2009, 131, 14290-14298.	13.7	124
46	Verdict: Time-Dependent Density Functional Theory â€œNot Guiltyâ€•of Large Errors for Cyanines. Journal of Chemical Theory and Computation, 2012, 8, 1255-1259.	5.3	122
47	Assessment of long-range corrected functionals performance for nâ†'Ï€* transitions in organic dyes. Journal of Chemical Physics, 2007, 127, 094102.	3.0	119
48	Accurate Evaluation of Valence and Low-Lying Rydberg States with Standard Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2007, 111, 5549-5556.	2.5	119
49	Contribution to the Mechanism of Copper-Catalyzed Câ€“N and Câ€“O Bond Formation. Organometallics, 2012, 31, 7694-7707.	2.3	119
50	Exploring excited states using Time Dependent Density Functional Theory and density-based indexes. Coordination Chemistry Reviews, 2015, 304-305, 166-178.	18.8	118
51	Accurate excitation energies from time-dependent density functional theory: assessing the PBE0 model for organic free radicals. Chemical Physics Letters, 1999, 314, 152-157.	2.6	116
52	A General Guidebook for the Theoretical Prediction of Physicochemical Properties of Chemicals for Regulatory Purposes. Chemical Reviews, 2015, 115, 13093-13164.	47.7	116
53	Time-dependent density functional theory investigation of the absorption, fluorescence, and phosphorescence spectra of solvated coumarins. Journal of Chemical Physics, 2006, 125, 164324.	3.0	115
54	Communication: One third: A new recipe for the PBE0 paradigm. Journal of Chemical Physics, 2013, 138, 021104.	3.0	115

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55	The meta-GGA functional: Thermochemistry with a kinetic energy density dependent exchange-correlation functional. Journal of Chemical Physics, 2000, 112, 2643-2649.	3.0	114
56	TD-DFT Vibronic Couplings in Anthraquinones: From Basis Set and Functional Benchmarks to Applications for Industrial Dyes. Journal of Chemical Theory and Computation, 2011, 7, 1882-1892.	5.3	113
57	Electronic Excitations in Solution: The Interplay between State Specific Approaches and a Time-Dependent Density Functional Theory Description. Journal of Chemical Theory and Computation, 2015, 11, 5782-5790.	5.3	112
58	Surface-dependent oxidation of H 2 on CeO 2 surfaces. Journal of Catalysis, 2013, 297, 193-201.	6.2	109
59	Phototriggered Linkage Isomerization in Rutheniumâ˜Dimethylsulfoxyde Complexes:Â Insights from Theory. Journal of Physical Chemistry A, 2003, 107, 11182-11190.	2.5	108
60	Spectroscopic Properties of Porphyrin-Like Photosensitizers:Â Insights from Theory. Journal of Physical Chemistry B, 2006, 110, 2398-2404.	2.6	106
61	Modeling Dye-Sensitized Solar Cells: From Theory to Experiment. Journal of Physical Chemistry Letters, 2013, 4, 1044-1050.	4.6	104
62	Nonempirical Double-Hybrid Functionals: An Effective Tool for Chemists. Accounts of Chemical Research, 2016, 49, 1503-1513.	15.6	103
63	Performance of the `parameter free' PBE0 functional for the modeling of molecular properties of heavy metals. Chemical Physics Letters, 2000, 325, 99-105.	2.6	100
64	Orthorhombic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 109, 247606.	7.8	100
65	Double-hybrid density functionals: merging wavefunction and density approaches to get the best of both worlds. Physical Chemistry Chemical Physics, 2013, 15, 14581.	2.8	100
66	Proton transfer in model hydrogen-bonded systems by a density functional approach. Chemical Physics Letters, 1994, 231, 295-300.	2.6	99
67	A hybrid density functional study of the firstâ€row transitionâ€metal monocarbonyls. Journal of Chemical Physics, 1995, 103, 10605-10613.	3.0	99
68	Comment on â€œAbout the calculation of exchange coupling constants using density-functional theory: The role of the self-interaction errorâ€•[J. Chem. Phys. 123, 164110 (2005)]. Journal of Chemical Physics, 2006, 124, 107101.	3.0	99
69	Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. Journal of Chemical Physics, 2012, 136, 174103.	3.0	99
70	Extensive TD-DFT investigation of the first electronic transition in substituted azobenzenes. Chemical Physics Letters, 2008, 465, 226-229.	2.6	96
71	Is the Tamm-Dancoff Approximation Reliable for the Calculation of Absorption and Fluorescence Band Shapes?. Journal of Chemical Theory and Computation, 2013, 9, 4517-4525.	5.3	95
72	Density Functional Study of Intrinsic and Environmental Effects in the Tautomeric Equilibrium of 2-Pyridone. The Journal of Physical Chemistry, 1995, 99, 15062-15068.	2.9	94

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73	A Theoretical Study of Bonding in Lanthanide Trihalides by Density Functional Methods. Journal of Physical Chemistry A, 1998, 102, 6812-6820.	2.5	94
74	Communication: Rationale for a new class of double-hybrid approximations in density-functional theory. Journal of Chemical Physics, 2011, 135, 101102.	3.0	93
75	Implementation and validation of the Lacks-Gordon exchange functional in conventional density functional and adiabatic connection methods. Journal of Computational Chemistry, 1998, 19, 418-429.	3.3	91
76	Comparative studies of quasi-relativistic density functional methods for the description of lanthanide and actinide complexes. Journal of Computational Chemistry, 2003, 24, 850-858.	3.3	89
77	Localized Excited Charge Carriers Generate Ultrafast Inhomogeneous Strain in the Multiferroic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>BiFeO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn</mml:mrow> Physical Review Letters, 2014, 112, 097602.	7.8	89
78	Accurate static polarizabilities by density functional theory: assessment of the PBE0 model. Chemical Physics Letters, 1999, 307, 265-271.	2.6	86
79	DFT and Proton Transfer Reactions: A Benchmark Study on Structure and Kinetics. Journal of Chemical Theory and Computation, 2012, 8, 3082-3088.	5.3	85
80	Validation and assessment of an accurate approach to the correlation problem in density functional theory: The Krigerâ€“Chenâ€“Iafrateâ€“Savin model. Journal of Chemical Physics, 2002, 117, 10465-10473.	3.0	83
81	Theoretical study of direct and water-assisted isomerization of formaldehyde radical cation. A comparison between density functional and post-Hartree-Fock approaches. Chemical Physics Letters, 1994, 224, 432-438.	2.6	82
82	Impact of Vibronic Couplings on Perceived Colors: Two Anthraquinones as a Working Example. Journal of Physical Chemistry Letters, 2012, 3, 468-471.	4.6	82
83	Predictions of Optical Excitations in Transition-Metal Complexes with Time Dependent-Density Functional Theory:Â Influence of Basis Sets. Journal of Chemical Theory and Computation, 2005, 1, 953-962.	5.3	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:Â Insights from Theory. Inorganic Chemistry, 2006, 45, 8517-8522.	4.0	77
85	Assessment of Several Hybrid DFT Functionals for the Evaluation of Bond Length Alternation of Increasingly Long Oligomers. Journal of Physical Chemistry A, 2006, 110, 5952-5959.	2.5	77
86	Absorption Spectra of First-Row Transition Metal Complexes of Bacteriochlorins:â€‰ A Theoretical Analysis. Journal of Physical Chemistry B, 2005, 109, 12214-12221.	2.6	76
87	A Comprehensive Theoretical View of the Bonding in Actinide Molecular Complexes. Journal of the American Chemical Society, 2006, 128, 2190-2191.	13.7	76
88	On the TD-DFT Accuracy in Determining Single and Double Bonds in Excited-State Structures of Organic Molecules. Journal of Physical Chemistry A, 2010, 114, 13402-13410.	2.5	76
89	Ab Initio Molecular Dynamics Study of a Highly Concentrated LiCl Aqueous Solution. Journal of Chemical Theory and Computation, 2008, 4, 1040-1048.	5.3	74
90	Accuracy of TD-DFT Geometries: A Fresh Look. Journal of Chemical Theory and Computation, 2018, 14, 3715-3727.	5.3	74

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91	Oxidation mechanism of diethyl ether: a complex process for a simple molecule. Physical Chemistry Chemical Physics, 2011, 13, 14636.	2.8	73
92	Theoretical Unraveling of Selective 1-Butene Oligomerization Catalyzed by Ironâ^'Bis(arylimino)pyridine. Organometallics, 2009, 28, 5358-5367.	2.3	72
93	Insights into Working Principles of Ruthenium Polypyridyl Dye-Sensitized Solar Cells from First Principles Modeling. Journal of Physical Chemistry C, 2011, 115, 4297-4306.	3.1	71
94	Absorption and emission spectra in gas-phase and solution using TD-DFT: Formaldehyde and benzene as case studies. Chemical Physics Letters, 2006, 421, 272-276.	2.6	70
95	Evaluating pushâ€“pull dye efficiency using TD-DFT and charge transfer indices. Physical Chemistry Chemical Physics, 2013, 15, 20210.	2.8	68
96	Functionalized Graphene as an Electronâ€Cascade Acceptor for Airâ€Processed Organic Ternary Solar Cells. Advanced Functional Materials, 2015, 25, 3870-3880.	14.9	67
97	Ionic versus covalent character in lanthanide complexes. A hybrid density functional study. Chemical Physics Letters, 1997, 268, 61-68.	2.6	66
98	First-row transition-metal hydrides: A challenging playground for new theoretical approaches. International Journal of Quantum Chemistry, 1997, 61, 443-451.	2.0	65
99	Theoretical Study of the Addition of Hydrogen Cyanide to Methanimine in the Gas Phase and in Aqueous Solution. Journal of the American Chemical Society, 2000, 122, 324-330.	13.7	65
100	Complete structural and magnetic characterization of biological radicals in solution by an integrated quantum mechanical approach: Glycyl radical as a case study. Journal of Chemical Physics, 2004, 121, 6710-6718.	3.0	65
101	Designing Multifunctional Expanded Pyridiniums: Properties of Branched and Fused Head-to-Tail Bipyridiniums. Journal of the American Chemical Society, 2010, 132, 16700-16713.	13.7	65
102	The geometries, absorption and fluorescence wavelengths of solvated fluorescent coumarins: A CIS and TD-DFT comparative study. Chemical Physics Letters, 2007, 438, 208-212.	2.6	63
103	Effective electron displacements: A tool for time-dependent density functional theory computational spectroscopy. Journal of Chemical Physics, 2014, 140, 104101.	3.0	63
104	A comprehensive DFT investigation of bulk and low-index surfaces of ZrO₂polymorphs. Journal of Computational Chemistry, 2015, 36, 9-21.	3.3	61
105	Range-separated hybrid density functionals made simple. Journal of Chemical Physics, 2019, 150, 201102.	3.0	60
106	Theoretical Insights on O2and CO Adsorption on Neutral and Positively Charged Gold Clusters. Journal of Physical Chemistry B, 2006, 110, 12240-12248.	2.6	58
107	Absorption and emission spectra of 1,8-naphthalimide fluorophores: A PCM-TD-DFT investigation. Chemical Physics, 2010, 372, 61-66.	1.9	58
108	Structure and magnetic properties of benzyl, anilino, and phenoxyl radicals by density functional computations. Journal of Chemical Physics, 1998, 109, 10244-10254.	3.0	57

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109	Spectral properties of self-assembled squaraineâ€“tetralactam: a theoretical assessment. Physical Chemistry Chemical Physics, 2009, 11, 1258.	2.8	57
110	Excited-State Geometries of Heteroaromatic Compounds: A Comparative TD-DFT and SAC-CI Study. Journal of Chemical Theory and Computation, 2013, 9, 2368-2379.	5.3	57
111	The nature of vertical excited states of dyes containing metals for DSSC applications: insights from TD-DFT and density based indexes. Physical Chemistry Chemical Physics, 2014, 16, 14435.	2.8	57
112	Theoretical Exploration of Type I/Type II Dual Photoreactivity of Promising Ru(II) Dyads for PDT Approach. Inorganic Chemistry, 2016, 55, 11185-11192.	4.0	57
113	Theoretical Investigation on the Role of the Central Carbon Atom and Close Protein Environment on the Nitrogen Reduction in Mo Nitrogenase. ACS Catalysis, 2016, 6, 1567-1577.	11.2	57
114	Density functional approach to the structures and EPR parameters of open shell systems. The case of fluorovinyl radicals. Chemical Physics Letters, 1993, 212, 5-11.	2.6	56
115	On the TD-DFT UV/vis spectra accuracy: the azoalkanes. Theoretical Chemistry Accounts, 2008, 120, 405-410.	1.4	56
116	A new parameter-free correlation functional based on an average atomic reduced density gradient analysis. Journal of Chemical Physics, 2008, 128, 034101.	3.0	56
117	From Classical Density Functionals to Adiabatic Connection Methods. The State of the Art.. Advances in Quantum Chemistry, 2000, 36, 45-75.	0.8	53
118	Understanding Aggregation-Induced Emission in Molecular Crystals: Insights from Theory. Journal of Physical Chemistry C, 2017, 121, 5747-5752.	3.1	52
119	Assessment of recently developed density functional approaches for the evaluation of the bond length alternation in polyacetylene. Chemical Physics Letters, 2005, 405, 376-381.	2.6	51
120	Exploring the Metric of Excited State Proton Transfer Reactions. Journal of Physical Chemistry B, 2013, 117, 16165-16173.	2.6	51
121	Performance of the Ï„-dependent functionals in predicting the magnetic coupling of ionic antiferromagnetic insulators. Journal of Chemical Physics, 2004, 120, 3811-3816.	3.0	50
122	Self-interaction error in density functional theory: a mean-field correction for molecules and large systems. Chemical Physics, 2005, 309, 67-76.	1.9	50
123	Morphological and charge transport properties of amorphous and crystalline P3HT and PBTTT: insights from theory. Physical Chemistry Chemical Physics, 2015, 17, 18742-18750.	2.8	50
124	Transport properties in manganite thin films. Physical Review B, 2005, 71, .	3.2	49
125	A mean-field self-interaction correction in density functional theory: implementation and validation for molecules. Chemical Physics Letters, 2003, 380, 12-20.	2.6	48
126	Solvent effects on an SN2 reaction profile. Chemical Physics Letters, 1998, 297, 1-7.	2.6	46

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127	Density Functional Study of Diborane, Dialane, and Digallane. The Journal of Physical Chemistry, 1994, 98, 13185-13188.	2.9	45
128	Theoretical Study of the Decomposition Reactions in Substituted Nitrobenzenes. Journal of Physical Chemistry A, 2008, 112, 4054-4059.	2.5	45
129	Range-Separated Double-Hybrid Functional from Nonempirical Constraints. Journal of Chemical Theory and Computation, 2018, 14, 4052-4062.	5.3	45
130	Comparison of convetional and hybrid density functional approaches. Cationic hydrides of first-row transition metals as a case study. Chemical Physics Letters, 1996, 249, 290-296.	2.6	44
131	Catalytic and bulk solvent effects on proton transfer: Formamide as a case study. Journal of Computational Chemistry, 1997, 18, 1993-2000.	3.3	44
132	Intramolecular Spin Alignment in Photomagnetic Molecular Devices: A Theoretical Study. Chemistry - A European Journal, 2007, 13, 5360-5377.	3.3	44
133	Computational Protocol for Modeling Thermochromic Molecular Crystals: Salicylidene Aniline As a Case Study. Journal of Chemical Theory and Computation, 2014, 10, 5577-5585.	5.3	44
134	Electronic Band Shapes Calculated with Optimally Tuned Range-Separated Hybrid Functionals. Journal of Chemical Theory and Computation, 2014, 10, 4599-4608.	5.3	44
135	Non-radiative decay paths in rhodamines: new theoretical insights. Physical Chemistry Chemical Physics, 2014, 16, 20681-20688.	2.8	44
136	Theoretical Investigation of Hole Transporter Materials for Energy Devices. Journal of Physical Chemistry C, 2015, 119, 23890-23898.	3.1	44
137	Systematic Improvement of Density Functionals through Parameter-Free Hybridization Schemes. Journal of Physical Chemistry Letters, 2015, 6, 3540-3545.	4.6	44
138	Charge transfer excitations in TDDFT: A ghostâ€hunter index. Journal of Computational Chemistry, 2017, 38, 2151-2156.	3.3	44
139	Photoinduced Processes within Compact Dyads Based on Triphenylpyridinium-Functionalized Bipyridyl Complexes of Ruthenium(II). Chemistry - A European Journal, 2005, 11, 3711-3727.	3.3	43
140	Fluorescence of 1,8-naphthalimide: A PCM-TD-DFT investigation. Chemical Physics Letters, 2007, 448, 3-6.	2.6	43
141	Modeling ZnO phases using a periodic approach: From bulk to surface and beyond. Journal of Chemical Physics, 2009, 131, 044708.	3.0	43
142	A Theoretical Study of the Decomposition Mechanisms in Substituted o-Nitrotoluenes. Journal of Physical Chemistry A, 2009, 113, 13621-13627.	2.5	43
143	The ammonium nitrate and its mechanism of decomposition in the gas phase: a theoretical study and a DFT benchmark. Physical Chemistry Chemical Physics, 2013, 15, 10849.	2.8	43
144	Structure and ESR features of glycine radical in its zwitterionic form. Chemical Physics Letters, 1995, 242, 351-354.	2.6	42

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145	Bi-isonicotinic Acid on Anatase (101):â€‰ Insights from Theory. Journal of Physical Chemistry C, 2007, 111, 15034-15042.	3.1	42
146	Phosphorescent Binuclear Iridium Complexes Based on Terpyridineâ€“Carboxylate: An Experimental and Theoretical Study. Inorganic Chemistry, 2011, 50, 8197-8206.	4.0	42
147	Influence of the Formation of the Halogen Bond ArX-â€‰-â€‰-N on the Mechanism of Diketonate Ligated Copper-Catalyzed Amination of Aromatic Halides. Organometallics, 2012, 31, 914-920.	2.3	42
148	Double hybrids and timeâ€dependent density functional theory: An implementation and benchmark on charge transfer excited states. Journal of Computational Chemistry, 2020, 41, 1242-1251.	3.3	42
149	A reliable method for fitting TD-DFT transitions to experimental UVâ€“visible spectra. Computational and Theoretical Chemistry, 2010, 954, 52-56.	1.5	41
150	Application of recent double-hybrid density functionals to low-lying singlet-singlet excitation energies of large organic compounds. Journal of Chemical Physics, 2013, 139, 164104.	3.0	41
151	Prediction of the thermal decomposition of organic peroxides by validated QSPR models. Journal of Hazardous Materials, 2014, 276, 216-224.	12.4	41
152	Characterizing Agosticity Using the Quantum Theory of Atoms in Molecules: Bond Critical Points and Their Local Properties. Journal of Physical Chemistry A, 2012, 116, 5472-5479.	2.5	40
153	B,Nâ€Codoped graphene as catalyst for the oxygen reduction reaction: Insights from periodic and cluster DFT calculations. Journal of Computational Chemistry, 2018, 39, 637-647.	3.3	39
154	Aggregation-caused quenching versus crystallization induced emission in thiazolo[5,4-b]thieno[3,2-e]pyridine (TTP) derivatives: theoretical insights. Physical Chemistry Chemical Physics, 2019, 21, 46-56.	2.8	39
155	Structures and properties of lanthanide and actinide complexes by a new density functional approach: Lanthanum, gadolinium, lutetium, and thorium halides as case studies. Journal of Computational Chemistry, 2000, 21, 1153-1166.	3.3	38
156	Evidence for the Iron(III) Oxidation State in Bis(imino)pyridine Catalysts. A Density Functional Theory Study. Organometallics, 2008, 27, 3368-3377.	2.3	38
157	Absorption spectra of azobenzenes simulated with timeâ€dependent density functional theory. International Journal of Quantum Chemistry, 2011, 111, 4224-4240.	2.0	38
158	Describing Excited State Intramolecular Proton Transfer in Dual Emissive Systems: A Density Functional Theory Based Analysis. Journal of Physical Chemistry B, 2015, 119, 2459-2466.	2.6	38
159	CO Oxidation on Cationic Gold Clusters: A Theoretical Study. Journal of Physical Chemistry C, 2008, 112, 18061-18066.	3.1	37
160	On the prediction of thermal stability of nitroaromatic compounds using quantum chemical calculations. Journal of Hazardous Materials, 2009, 171, 845-850.	12.4	37
161	Is There Still Room for Parameter Free Double Hybrids? Performances of PBE0-DH and B2PLYP over Extended Benchmark Sets. Journal of Chemical Theory and Computation, 2013, 9, 3444-3452.	5.3	37
162	Density functional theory: An effective theoretical tool for the study of ? radicals. International Journal of Quantum Chemistry, 1994, 52, 963-971.	2.0	36

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163	Low temperature magnetism in the perovskite substrate DyScO3. Applied Physics Letters, 2009, 94, .	3.3	36
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