Ilaria Ciofini

List of Publications by Citations

234 papers	10,226 citations	50 h-index	91 g-index
258 ext. papers	11,155 ext. citations	5.4 avg, IF	6.41 L-index

#	Paper	IF	Citations
234	TD-DFT Performance for the Visible Absorption Spectra of Organic Dyes: Conventional versus Long-Range Hybrids. *Journal of Chemical Theory and Computation*, **2008**, 4, 123-35	6.4	681
233	A Qualitative Index of Spatial Extent in Charge-Transfer Excitations. *Journal of Chemical Theory and Computation*, **2011**, 7, 2498-506	6.4	657
232	Accurate simulation of optical properties in dyes. *Accounts of Chemical Research*, **2009**, 42, 326-34	24.3	404
231	On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies. *Journal of Chemical Theory and Computation*, **2010**, 6, 2071-85	6.4	335
230	Mechanism of the palladium-catalyzed homocoupling of arylboronic acids: key involvement of a palladium peroxo complex. *Journal of the American Chemical Society*, **2006**, 128, 6829-36	16.4	313
229	What is the "best" atomic charge model to describe through-space charge-transfer excitations?. *Physical Chemistry Chemical Physics*, **2012**, 14, 5383-8	3.6	242
228	Photoinduced intramolecular electron transfer in ruthenium and osmium polyads: insights from theory. *Journal of the American Chemical Society*, **2004**, 126, 10763-77	16.4	195
227	Through-Space Charge Transfer in Rod-Like Molecules: Lessons from Theory. *Journal of Physical Chemistry C*, **2012**, 116, 11946-11955	3.8	193
226	First-principles modeling of dye-sensitized solar cells: challenges and perspectives. *Accounts of Chemical Research*, **2012**, 45, 1268-77	24.3	182
225	Assessment of Functionals for TD-DFT Calculations of Singlet-Triplet Transitions. *Journal of Chemical Theory and Computation*, **2010**, 6, 1532-7	6.4	173
224	DFT calculations of molecular magnetic properties of coordination compounds. *Coordination Chemistry Reviews*, **2003**, 238-239, 187-209	23.2	170
223	On the Calculation and Modeling of Magnetic Exchange Interactions in Weakly Bonded Systems: The Case of the Ferromagnetic Copper(II) &mgr;(2)-Azido Bridged Complexes. *Inorganic Chemistry*, **1999**, 38, 1996-2004	5.1	154
222	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, 11276-84	3.6	144
221	Wavelength-Emission Tuning of ZnO Nanowire-Based Light-Emitting Diodes by Cu Doping: Experimental and Computational Insights. *Advanced Functional Materials*, **2011**, 21, 3564-3572	15.6	138
220	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, 14290-8	16.4	120
219	Assessment of the B97 family for excited-state calculations. *Theoretical Chemistry Accounts*, **2011**, 128, 127-136	1.9	115
218	Verdict: Time-Dependent Density Functional Theory "Not Guilty" of Large Errors for Cyanines. *Journal of Chemical Theory and Computation*, **2012**, 8, 1255-9	6.4	110

217	Accurate evaluation of valence and low-lying Rydberg states with standard time-dependent density functional theory. *Journal of Physical Chemistry A*, **2007**, 111, 5549-56	2.8	104
216	Time-dependent density functional theory investigation of the absorption, fluorescence, and phosphorescence spectra of solvated coumarins. *Journal of Chemical Physics*, **2006**, 125, 164324	3.9	104
215	Transition-Metal-Free Arylation of Enolizable Aryl Ketones and Mechanistic Evidence for a Radical Process. *Angewandte Chemie - International Edition*, **2015**, 54, 10587-91	16.4	101
214	Contribution to the Mechanism of Copper-Catalyzed CN and CO Bond Formation. *Organometallics*, **2012**, 31, 7694-7707	3.8	101
213	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, 1882-92	6.4	96
212	Exploring excited states using Time Dependent Density Functional Theory and density-based indexes. *Coordination Chemistry Reviews*, **2015**, 304-305, 166-178	23.2	94
211	Phototriggered Linkage Isomerization in RutheniumDimethylsulfoxyde Complexes:Insights from Theory. *Journal of Physical Chemistry A*, **2003**, 107, 11182-11190	2.8	94
210	Modeling Dye-Sensitized Solar Cells: From Theory to Experiment. *Journal of Physical Chemistry Letters*, **2013**, 4, 1044-50	6.4	93
209	Ultra-sensitive and selective hydrogen nanosensor with fast response at room temperature based on a single Pd/ZnO nanowire. *Sensors and Actuators B: Chemical*, **2018**, 254, 1259-1270	8.5	91
208	Extensive TD-DFT investigation of the first electronic transition in substituted azobenzenes. *Chemical Physics Letters*, **2008**, 465, 226-229	2.5	88
207	Rationally designed ruthenium complexes for 1- and 2-photon photodynamic therapy. *Nature Communications*, **2020**, 11, 3262	17.4	83
206	Theoretical procedure for optimizing dye-sensitized solar cells: from electronic structure to photovoltaic efficiency. *Journal of the American Chemical Society*, **2011**, 133, 8005-13	16.4	80
205	Ground and Excited State Properties and Vibronic Coupling Analysis of the CreutzTaube Ion, [(NH3)5Ru-pyrazine-Ru(NH3)5]5+, Using DFT. *Journal of the American Chemical Society*, **1999**, 121, 11418-11424	16.4	75
204	Nonempirical Double-Hybrid Functionals: An Effective Tool for Chemists. *Accounts of Chemical Research*, **2016**, 49, 1503-13	24.3	75
203	Rationally Designed Long-Wavelength Absorbing Ru(II) Polypyridyl Complexes as Photosensitizers for Photodynamic Therapy. *Journal of the American Chemical Society*, **2020**, 142, 6578-6587	16.4	74
202	Assessment of several hybrid DFT functionals for the evaluation of bond length alternation of increasingly long oligomers. *Journal of Physical Chemistry A*, **2006**, 110, 5952-9	2.8	71
201	Impact of Vibronic Couplings on Perceived Colors: Two Anthraquinones as a Working Example. *Journal of Physical Chemistry Letters*, **2012**, 3, 468-71	6.4	69
200	Effect of solvent and additives on the open-circuit voltage of ZnO-based dye-sensitized solar cells: a combined theoretical and experimental study. *Physical Chemistry Chemical Physics*, **2010**, 12, 14710-9	3.6	67

199	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	2.5	66
198	Insights into Working Principles of Ruthenium Polypyridyl Dye-Sensitized Solar Cells from First Principles Modeling. *Journal of Physical Chemistry C*, **2011**, 115, 4297-4306	3.8	64
197	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, 6710-8	3.9	64
196	High Aspect Ratio Ternary Zn1−xCdxO Nanowires by Electrodeposition for Light-Emitting Diode Applications. *Journal of Physical Chemistry C*, **2011**, 115, 14548-14558	3.8	61
195	Correct dissociation behavior of radical ions such as H2+ in density functional calculations. *Journal of Chemical Physics*, **2001**, 114, 1447-1453	3.9	60
194	Revealing the Origins of Mechanically Induced Fluorescence Changes in Organic Molecular Crystals. *Advanced Materials*, **2018**, 30, e1800817	24	58
193	Designing multifunctional expanded pyridiniums: properties of branched and fused head-to-tail bipyridiniums. *Journal of the American Chemical Society*, **2010**, 132, 16700-13	16.4	55
192	Multifrequency EPR study and density functional g-tensor calculations of persistent organorhenium radical complexes. *Journal of the American Chemical Society*, **2002**, 124, 10563-71	16.4	55
191	Two-electron versus one-electron reduction of chalcogens by uranium(III): synthesis of a terminal U(V) persulfide complex. *Chemical Science*, **2014**, 5, 841-846	9.4	54
190	Excited-State Geometries of Heteroaromatic Compounds: A Comparative TD-DFT and SAC-CI Study. *Journal of Chemical Theory and Computation*, **2013**, 9, 2368-79	6.4	54
189	Theoretical insights on O2 and CO adsorption on neutral and positively charged gold clusters. *Journal of Physical Chemistry B*, **2006**, 110, 12240-8	3.4	54
188	Evaluating push-pull dye efficiency using TD-DFT and charge transfer indices. *Physical Chemistry Chemical Physics*, **2013**, 15, 20210-9	3.6	53
187	Low-Temperature Preparation of Ag-Doped ZnO Nanowire Arrays, DFT Study, and Application to Light-Emitting Diode. *ACS Applied Materials & Interfaces*, **2015**, 7, 11871-80	9.5	53
186	Absorption and emission spectra of 1,8-naphthalimide fluorophores: A PCM-TD-DFT investigation. *Chemical Physics*, **2010**, 372, 61-66	2.3	53
185	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, 14435-44	3.6	51
184	Exploring the metric of excited state proton transfer reactions. *Journal of Physical Chemistry B*, **2013**, 117, 16165-73	3.4	50
183	On the TD-DFT UV/vis spectra accuracy: the azoalkanes. *Theoretical Chemistry Accounts*, **2008**, 120, 405-410	1.9	50
182	Taming Nickel-Catalyzed Suzuki-Miyaura Coupling: A Mechanistic Focus on Boron-to-Nickel Transmetalation. *ACS Catalysis*, **2018**, 8, 4812-4823	13.1	49

181	Performance of the tau-dependent functionals in predicting the magnetic coupling of ionic antiferromagnetic insulators. *Journal of Chemical Physics*, **2004**, 120, 3811-6	3.9	49
180	A posteriori corrections to systematic failures of standard density functionals: The dissociation of two-center three-electron systems. *Journal of Chemical Physics*, **2001**, 115, 11068-11079	3.9	48
179	Self-interaction error in density functional theory: a mean-field correction for molecules and large systems. *Chemical Physics*, **2005**, 309, 67-76	2.3	47
178	Assessment of recently developed density functional approaches for the evaluation of the bond length alternation in polyacetylene. *Chemical Physics Letters*, **2005**, 405, 376-381	2.5	47
177	A mean-field self-interaction correction in density functional theory: implementation and validation for molecules. *Chemical Physics Letters*, **2003**, 380, 12-20	2.5	45
176	Occurence of abundant diradicaloid moieties in the insoluble organic matter from the Orgueil and Murchison meteorites: a fingerprint of its extraterrestrial origin?. *Geochimica Et Cosmochimica Acta*, **2004**, 68, 881-891	5.5	45
175	Density Functional Modeling of Double Exchange Interactions in Transition Metal Complexes. Calculation of the Ground and Excited State Properties of [Fe2(OH)3(tmtacn)2]2+. *Journal of the American Chemical Society*, **1998**, 120, 8357-8365	16.4	45
174	Multiconfiguration Pair-Density Functional Theory Predicts Spin-State Ordering in Iron Complexes with the Same Accuracy as Complete Active Space Second-Order Perturbation Theory at a Significantly Reduced Computational Cost. *Journal of Physical Chemistry Letters*, **2017**, 8, 2026-2030	6.4	43
173	Modeling ZnO phases using a periodic approach: from bulk to surface and beyond. *Journal of Chemical Physics*, **2009**, 131, 044708	3.9	43
172	Phosphorescent binuclear iridium complexes based on terpyridine-carboxylate: an experimental and theoretical study. *Inorganic Chemistry*, **2011**, 50, 8197-206	5.1	42
171	Intramolecular spin alignment in photomagnetic molecular devices: a theoretical study. *Chemistry - A European Journal*, **2007**, 13, 5360-77	4.8	42
170	Solvent effects on g-tensors of semiquinone radical anions: polarizable continuum versus cluster models. *Theoretical Chemistry Accounts*, **2004**, 111, 132-140	1.9	42
169	Influence of the Formation of the Halogen Bond ArX- - -N on the Mechanism of Diketonate Ligated Copper-Catalyzed Amination of Aromatic Halides. *Organometallics*, **2012**, 31, 914-920	3.8	41
168	Expanded pyridiniums: bis-cyclization of branched pyridiniums into their fused polycyclic and positively charged derivatives--assessing the impact of pericondensation on structural, electrochemical, electronic, and photophysical features. *Chemistry - A European Journal*, **2010**, 16, 11047-63	4.8	40
167	Fluorescence of 1,8-naphthalimide: A PCM-TD-DFT investigation. *Chemical Physics Letters*, **2007**, 448, 3-6	2.5	40
166	Morphological and charge transport properties of amorphous and crystalline P3HT and PBTTT: insights from theory. *Physical Chemistry Chemical Physics*, **2015**, 17, 18742-50	3.6	39
165	Red-light-driven photocatalytic hydrogen evolution using a ruthenium quaterpyridine complex. *Chemical Communications*, **2015**, 51, 9261-4	5.8	39
164	Computational Protocol for Modeling Thermochromic Molecular Crystals: Salicylidene Aniline As a Case Study. *Journal of Chemical Theory and Computation*, **2014**, 10, 5577-85	6.4	39

163	Photoinduced processes within compact dyads based on triphenylpyridinium-functionalized bipyridyl complexes of ruthenium(II). *Chemistry - A European Journal*, **2005**, 11, 3711-27	4.8	39
162	Understanding Aggregation-Induced Emission in Molecular Crystals: Insights from Theory. *Journal of Physical Chemistry C*, **2017**, 121, 5747-5752	3.8	37
161	Theoretical Investigation of Hole Transporter Materials for Energy Devices. *Journal of Physical Chemistry C*, **2015**, 119, 23890-23898	3.8	37
160	Describing excited state intramolecular proton transfer in dual emissive systems: a density functional theory based analysis. *Journal of Physical Chemistry B*, **2015**, 119, 2459-66	3.4	37
159	CO Oxidation on Cationic Gold Clusters: A Theoretical Study. *Journal of Physical Chemistry C*, **2008**, 112, 18061-18066	3.8	37
158	Comparison of structural dynamics and coherence of d-d and MLCT light-induced spin state trapping. *Chemical Science*, **2017**, 8, 4978-4986	9.4	35
157	Copper-Catalyzed Hydroamination of Allenes: from Mechanistic Understanding to Methodology Development. *ACS Catalysis*, **2017**, 7, 4253-4264	13.1	35
156	Non-radiative decay paths in rhodamines: new theoretical insights. *Physical Chemistry Chemical Physics*, **2014**, 16, 20681-8	3.6	35
155	Theoretical determination of the pKas of the 8-hydroxyquinoline-5-sulfonic acid: A DFT based approach. *Chemical Physics Letters*, **2009**, 472, 30-34	2.5	35
154	Structure and Magnetic Properties of Oxoverdazyl Radicals and Biradicals by an Integrated Computational Approach. *Journal of Physical Chemistry A*, **1999**, 103, 4275-4282	2.8	35
153	Acetylacetone, an interesting anchoring group for ZnO-based organic-inorganic hybrid materials: a combined experimental and theoretical study. *Langmuir*, **2011**, 27, 3442-50	4	34
152	Investigation of NLO properties of substituted (M)-tetrathia-[7]-helicenes by semiempirical and DFT methods. *International Journal of Quantum Chemistry*, **2003**, 91, 297-302	2.1	34
151	Intermolecular proton shuttling in excited state proton transfer reactions: insights from theory. *Physical Chemistry Chemical Physics*, **2014**, 16, 8661-6	3.6	33
150	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, 3444-52	6.4	33
149	Benchmark Study on the Triplet Excited-State Geometries and Phosphorescence Energies of Heterocyclic Compounds: Comparison Between TD-PBE0 and SAC-CI. *Journal of Chemical Theory and Computation*, **2014**, 10, 3969-79	6.4	32
148	Discriminating role of bases in diketonate copper(I)-catalyzed C-O couplings: phenol versus diarylether. *Dalton Transactions*, **2013**, 42, 5348-54	4.3	32
147	Absorption spectra of azobenzenes simulated with time-dependent density functional theory. *International Journal of Quantum Chemistry*, **2011**, 111, 4224-4240	2.1	32
146	Fast and reliable theoretical determination of pKa* for photoacids. *Journal of Physical Chemistry A*, **2008**, 112, 794-6	2.8	32

145	Pd-catalyzed homocoupling reaction of arylboronic acid: insights from density functional theory. *Journal of Physical Chemistry A*, **2008**, 112, 12896-903	2.8	32
144	Theoretical analysis of the electronic properties of N3 derivatives. *Journal of Physical Chemistry A*, **2007**, 111, 13106-11	2.8	31
143	Conformationally gated photoinduced processes within photosensitizer-acceptor dyads based on osmium(II) complexes with triarylpyridinio-functionalized terpyridyl ligands: insights from theoretical analysis. *Inorganic Chemistry*, **2006**, 45, 5538-51	5.1	31
142	Charge transfer excitations in TDDFT: A ghost-hunter index. *Journal of Computational Chemistry*, **2017**, 38, 2151-2156	3.5	30
141	Intrinsic and dynamical reaction pathways of an excited state proton transfer. *Journal of Physical Chemistry B*, **2015**, 119, 2650-7	3.4	30
140	Vibrational analysis of glycine radical: a comparative ab initio static and dynamic study. *Physical Chemistry Chemical Physics*, **2009**, 11, 4375-84	3.6	30
139	Effect of self-interaction error in the evaluation of the bond length alternation in trans-polyacetylene using density-functional theory. *Journal of Chemical Physics*, **2005**, 123, 121102	3.9	30
138	Low-Temperature Solution Synthesis of Au-Modified ZnO Nanowires for Highly Efficient Hydrogen Nanosensors. *ACS Applied Materials & Interfaces*, **2019**, 11, 32115-32126	9.5	29
137	Photophysical properties of NIR-emitting fluorescence probes: insights from TD-DFT. *Physical Chemistry Chemical Physics*, **2013**, 15, 10019-27	3.6	29
136	Photophysical properties of 8-hydroxyquinoline-5-sulfonic acid as a function of the pH: a TD-DFT investigation. *Journal of Physical Chemistry A*, **2010**, 114, 5932-9	2.8	29
135	Effects of Substituents on Transport Properties of Molecular Materials for Organic Solar Cells: A Theoretical Investigation. *Chemistry of Materials*, **2017**, 29, 673-681	9.6	28
134	A Ru(II) polypyridyl complex bearing aldehyde functions as a versatile synthetic precursor for long-wavelength absorbing photodynamic therapy photosensitizers. *Bioorganic and Medicinal Chemistry*, **2019**, 27, 2666-2675	3.4	28
133	Interfacial Engineering through Chloride-Functionalized Self-Assembled Monolayers for High-Performance Perovskite Solar Cells. *ACS Applied Materials & Interfaces*, **2020**, 12, 744-752	9.5	28
132	Reaching optimal light-induced intramolecular spin alignment within photomagnetic molecular device prototypes. *Chemistry - A European Journal*, **2008**, 14, 11385-405	4.8	27
131	Revisiting the relationship between the bond length alternation and the first hyperpolarizability with range-separated hybrid functionals. *Journal of Computational Chemistry*, **2008**, 29, 921-5	3.5	27
130	Functionalized Pd/ZnO Nanowires for Nanosensors. *Physica Status Solidi - Rapid Research Letters*, **2018**, 12, 1700321	2.5	27
129	Double hybrids and time-dependent density functional theory: An implementation and benchmark on charge transfer excited states. *Journal of Computational Chemistry*, **2020**, 41, 1242-1251	3.5	26
128	Mechanistic Insights into C?N Coupling Catalyzed by 1,3-Diketonate-Ligated Copper: Unprecedented Activation of Aryl Iodide. *ChemCatChem*, **2011**, 3, 305-309	5.2	26

127	EPR, ENDOR, and HYSCORE study of the structure and the stability of vanadyl-porphyrin complexes encapsulated in silica: potential paramagnetic biomarkers for the origin of life. *Journal of Physical Chemistry B*, **2010**, 114, 3714-25	3.4	26
126	A DFT investigation of CO oxidation over neutral and cationic gold clusters. *Computational and Theoretical Chemistry*, **2009**, 903, 34-40		26
125	Molecular dyads of ruthenium(II)- or osmium(II)-bis(terpyridine) chromophores and expanded pyridinium acceptors: equilibration between MLCT and charge-separated excited states. *Inorganic Chemistry*, **2013**, 52, 11944-55	5.1	25
124	A theoretical spectroscopy investigation of bifunctional platinum-bridged diarylethenes. *Chemical Physics Letters*, **2011**, 502, 77-81	2.5	25
123	Chemically intuitive indices for charge-transfer excitation based on SAC-CI and TD-DFT calculations. *Journal of Computational Chemistry*, **2013**, 34, 2498-501	3.5	24
122	Metrics for Molecular Electronic Excitations: A Comparison between Orbital- and Density-Based Descriptors. *Journal of Physical Chemistry A*, **2017**, 121, 7543-7549	2.8	24
121	Photoinduced electron transfer in Os(terpyridine)-biphenylene-(bi)pyridinium assemblies. *Inorganic Chemistry*, **2012**, 51, 5342-52	5.1	24
120	Single-step versus stepwise two-electron reduction of polyarylpyridiniums: insights from the steric switching of redox potential compression. *Journal of the American Chemical Society*, **2012**, 134, 2691-705	16.4	24
119	Amphiphilic acids as co-adsorbents of metal-free organic dyes for the efficient sensitization of nanostructured photoelectrode. *RSC Advances*, **2012**, 2, 11836	3.7	23
118	Theoretical insights into branched and fused expanded pyridiniums by the means of density functional theory. *Journal of Physical Chemistry A*, **2010**, 114, 8434-43	2.8	23
117	First-principle molecular dynamics of the Berry pseudorotation: insights on 19F NMR in SF4. *Journal of Chemical Physics*, **2004**, 120, 9167-74	3.9	23
116	Kinetics of Multielectron Transfers and Redox-Induced Structural Changes in N-Aryl-Expanded Pyridiniums: Establishing Their Unusual, Versatile Electrophoric Activity. *Journal of the American Chemical Society*, **2015**, 137, 11349-64	16.4	22
115	Facile One-Pot Synthesis of Ruthenium(II) Quaterpyridine-Based Photosensitizers for Photocatalyzed Hydrogen Production. *Inorganic Chemistry*, **2017**, 56, 9515-9524	5.1	22
114	Revisiting the importance of dye binding mode in dye-sensitized solar cells: a periodic viewpoint. *Journal of Materials Chemistry*, **2012**, 22, 12205		22
113	Confinement Effects on UV-Visible Absorption Spectra: β-Carotene Inside Carbon Nanotube as a Test Case. *Journal of Physical Chemistry Letters*, **2013**, 4, 1239-43	6.4	22
112	Environmental effects on electronic absorption spectra using DFT: An organic and positively charged fused polycyclic chromophore as a case study. *Computational and Theoretical Chemistry*, **2009**, 914, 94-99		22
111	Atypical Lone Pair-π Interaction with Quinone Methides in a Series of Imido-Ferrociphenol Anticancer Drug Candidates. *Angewandte Chemie - International Edition*, **2019**, 58, 8421-8425	16.4	21
110	Direct Spirocyclization from Keto-sulfonamides: An Approach to Azaspiro Compounds. *Organic Letters*, **2017**, 19, 5042-5045	6.2	21

109	Spectral properties of bipyridyl ligands by time-dependent density functional theory. *Chemical Physics Letters*, **2006**, 417, 445-451	2.5	21
108	Modeling emission features of salicylidene aniline molecular crystals: A QM/QMCapproach. *Journal of Computational Chemistry*, **2016**, 37, 861-70	3.5	21
107	Modelling photophysical properties of metal-organic frameworks: a density functional theory based approach. *Physical Chemistry Chemical Physics*, **2016**, 18, 25176-25182	3.6	20
106	Response Enhancement of Self-Powered Visible-Blind UV Photodetectors by Nanostructured Heterointerface Engineering. *Advanced Functional Materials*, **2019**, 29, 1903981	15.6	20
105	Visible spectrum of naphthazarin investigated through Time-Dependent Density Functional Theory. *Chemical Physics Letters*, **2010**, 493, 67-71	2.5	19
104	Comparison of theoretical approaches for computing the bond length alternation of polymethineimine. *Chemical Physics*, **2007**, 332, 79-85	2.3	19
103	Intrinsic and Environmental Effects on the Kinetic and Thermodynamics of Linkage Isomerization in Nitritopentaamminecobalt(III) Complex. *Journal of Physical Chemistry A*, **2001**, 105, 1086-1092	2.8	19
102	Electrostatic Embedding To Model the Impact of Environment on Photophysical Properties of Molecular Crystals: A Self-Consistent Charge Adjustment Procedure. *Journal of Chemical Theory and Computation*, **2016**, 12, 3316-24	6.4	19
101	Computational Insights into Excited-State Proton-Transfer Reactions in Azo and Azomethine Dyes. *ChemPhysChem*, **2015**, 16, 3966-73	3.2	18
100	Intramolecular spin alignment within mono-oxidized and photoexcited anthracene-based pi radicals as prototypical photomagnetic molecular devices: relationships between electrochemical, photophysical, and photochemical control pathways. *Chemistry - A European Journal*, **2009**, 15, 11210-20	4.8	18
99	How are the charge transfer descriptors affected by the quality of the underpinning electronic density?. *Journal of Computational Chemistry*, **2018**, 39, 735-742	3.5	17
98	Investigation of the bulk and surface properties of CdSe: insights from theory. *Physical Chemistry Chemical Physics*, **2014**, 16, 23251-9	3.6	17
97	On the absorption spectra of recently synthesized carbonyl dyes: TD-DFT insights. *Journal of Physical Chemistry A*, **2010**, 114, 9579-82	2.8	17
96	Mapping the many-electron generalised spin-exchange Hamiltonian to accurate post-HF calculations. *Chemical Physics*, **2005**, 309, 133-141	2.3	17
95	Multiple Roles of Isocyanides in Palladium-Catalyzed Imidoylative Couplings: A Mechanistic Study. *Chemistry - A European Journal*, **2016**, 22, 15491-15500	4.8	17
94	Non-parametrized functionals with empirical dispersion corrections: A happy match?. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	16
93	Communication: Evaluating non-empirical double hybrid functionals for spin-state energetics in transition-metal complexes. *Journal of Chemical Physics*, **2018**, 148, 041103	3.9	16
92	Anchoring groups for dyes in p-DSSC application: insights from DFT. *Journal of Molecular Modeling*, **2016**, 22, 289	2	16

91	Ligand-stabilized CdSe nanoplatelet hybrid structures with tailored geometric and electronic properties. New insights from theory. *RSC Advances*, **2014**, 4, 55980-55989	3.7	16
90	Modeling of charge transfer processes to understand photophysical signatures: The case of Rhodamine 110. *Chemical Physics Letters*, **2014**, 610-611, 148-152	2.5	16
89	Understanding the redox properties of dinuclear ruthenium(II) complexes by a joint experimental and theoretical analysis. *Dalton Transactions*, **2013**, 42, 5281-91	4.3	16
88	First Evidence of the Oxidative Addition of Fe0(N,N)2 to Aryl Halides: This Precondition Is Not a Guarantee of Efficient Iron-Catalysed C N Cross-Coupling Reactions. *European Journal of Organic Chemistry*, **2011**, 2011, 3768-3780	3.2	16
87	Unveiling the Reactivity of a Synthetic Mimic of the Oxygen Evolving Complex. *Journal of Physical Chemistry Letters*, **2016**, 7, 5015-5021	6.4	15
86	Copper-Catalyzed Hydroamination of N-Allenylazoles: Access to Amino-Substituted N-Vinylazoles. *Advanced Synthesis and Catalysis*, **2017**, 359, 4388-4392	5.6	15
85	Solvent tuned single molecule dual emission in protic solvents: effect of polarity and H-bonding. *Faraday Discussions*, **2015**, 185, 285-97	3.6	15
84	Tictoid expanded pyridiniums: assessing structural, electrochemical, electronic, and photophysical features. *Journal of Physical Chemistry A*, **2012**, 116, 7880-91	2.8	15
83	Theoretical study of absorption and emission properties of green and yellow emitting iridium(III) complexes. *Journal of Physical Chemistry A*, **2011**, 115, 11861-5	2.8	15
82	Theoretical modelling of photoactive molecular systems: insights using the Density Functional Theory. *Comptes Rendus Chimie*, **2006**, 9, 226-239	2.7	15
81	Copper-amyloid- complex may catalyze peroxynitrite production in brain: evidence from molecular modeling. *Physical Chemistry Chemical Physics*, **2014**, 16, 10169-74	3.6	14
80	Solvent-tuned dual emission: a structural and electronic interplay highlighting a novel planar ICT (OPICT). *Physical Chemistry Chemical Physics*, **2015**, 17, 7639-42	3.6	14
79	Comparing the performance of TD-DFT and SAC-CI methods in the description of excited states potential energy surfaces: An excited state proton transfer reaction as case study. *Journal of Computational Chemistry*, **2017**, 38, 1084-1092	3.5	13
78	Ethylene dimerization catalyzed by mixed phosphine-iminophosphorane nickel(II) complexes: a DFT investigation. *Journal of Molecular Modeling*, **2013**, 19, 2107-18	2	13
77	Exploring the photophysical behaviour of supramolecular systems: problems and perspectives. *Theoretical Chemistry Accounts*, **2006**, 116, 219-231	1.9	13
76	Optical properties of the dibenzothiazolylphenol molecular crystals through ONIOM calculations: the effect of the electrostatic embedding scheme. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	13
75	Theoretical approaches for predicting the color of rigid dyes in solution. *Journal of Computational Chemistry*, **2017**, 38, 998-1004	3.5	12
74	Enzymatic oxidation of ansa-ferrocifen leads to strong and selective thioredoxin reductase inhibition in vitro. *Journal of Inorganic Biochemistry*, **2016**, 165, 146-151	4.2	12

73	Assessing the performances of some recently proposed density functionals for the description of organometallic structures. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	12
72	Generalized gradient exchange functionals based on the gradient-regulated connection: a new member of the TCA family. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	12
71	Environment effects on the oxidation of thiols: cobalt phthalocyanine as a test case. *Chemical Physics Letters*, **2003**, 376, 690-697	2.5	12
70	Aggregation Effects on Pigment Coatings: Pigment Red 179 as a Case Study. *ACS Omega*, **2019**, 4, 20315-20323	3.9	12
69	A family of Ru(II) complexes built on a novel sexipyridine building block: synthesis, photophysical properties and the rare structural characterization of a triruthenium species. *Dalton Transactions*, **2015**, 44, 11551-61	4.3	11
68	A DFT study of magnetic interactions in photoswitchable systems. *Chemical Physics Letters*, **2012**, 542, 13-18	2.5	11
67	Quantifying electron delocalization in orthogonal channels: Theoretical investigation of □and □ aromaticity in [C6I6]2+ and [C6Cl6]2+. *Chemical Physics Letters*, **2007**, 435, 171-175	2.5	11
66	Reactivity of nitrobenzofurazan towards nucleophiles: Insights from DFT. *Chemical Physics Letters*, **2008**, 461, 16-20	2.5	11
65	A qualitative model to identify non-radiative decay channels: the spiropyran as case study. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	11
64	Quantifying partial hole-particle distance at the excited state: A revised version of the DCT index. *Chemical Physics Letters*, **2019**, 714, 81-86	2.5	11
63	General Density-Based Index to Analyze Charge Transfer Phenomena: From Models to Butterfly Molecules. *Journal of Chemical Theory and Computation*, **2020**, 16, 4543-4553	6.4	10
62	Using Density Based Indexes and Wave Function Methods for the Description of Excited States: Excited State Proton Transfer Reactions as a Test Case. *Journal of Physical Chemistry A*, **2018**, 122, 375-382	2.8	10
61	Vibrational behavior of tetrahedral d0 oxo-compounds: A theoretical study. *Chemical Physics Letters*, **2006**, 429, 52-57	2.5	10
60	Solvent effects on molecular reactivity descriptors: some test cases. *Theoretical Chemistry Accounts* , **2004**, 111, 188-195	1.9	10
59	Assessing challenging intra- and inter-molecular charge-transfer excitations energies with double-hybrid density functionals. *Journal of Computational Chemistry*, **2021**, 42, 970-981	3.5	10
58	Excited-State Proton Transfer and Intramolecular Charge Transfer in 1,3-Diketone Molecules. *ChemPhysChem*, **2016**, 17, 1530-8	3.2	10
57	Copper-Catalysed Hydroamination of N-Allenylsulfonamides: The Key Role of Ancillary Coordinating Groups. *Synthesis*, **2019**, 51, 1225-1234	2.9	10
56	Emissive Azobenzenes Delivered on a Silver Coordination Polymer. *Inorganic Chemistry*, **2018**, 57, 15009-15022	4.5	10

55	Stereoselective access to trisubstituted fluorinated alkenyl thioethers. *Catalysis Science and Technology*, **2017**, 7, 1921-1927	5.5	9
54	Electron Storage System Based on a Two-Way Inversion of Redox Potentials. *Journal of the American Chemical Society*, **2020**, 142, 5162-5176	16.4	9
53	Promising anchoring groups for ZnO-based hybrid materials: A periodic density functional theory investigation. *International Journal of Quantum Chemistry*, **2012**, 112, 2062-2071	2.1	9
52	Electronic spectrum of 2-pyridone+: Ab initio and time-dependent density functional calculations. *International Journal of Quantum Chemistry*, **2010**, 110, 498-504	2.1	9
51	Excited state tracking during the relaxation of coordination compounds. *Journal of Computational Chemistry*, **2019**, 40, 1420-1428	3.5	8
50	An electron density based analysis to establish the electronic adiabaticity of proton coupled electron transfer reactions. *Journal of Computational Chemistry*, **2020**, 41, 1835-1841	3.5	8
49	Piano-stool d 6 -rhodium(III) complexes of chelating pyridine-based ligands and their papain bioconjugates for the catalysis of transfer hydrogenation of aryl ketones in aqueous medium. *Journal of Molecular Catalysis B: Enzymatic*, **2015**, 122, 314-322		8
48	Combined Computational and Experimental Study of CdSeS/ZnS Nanoplatelets: Structural, Vibrational, and Electronic Aspects of Core-Shell Interface Formation. *Langmuir*, **2018**, 34, 13828-13836	4	8
47	Supramolecular Anchoring of NCN-Pincer Palladium Complexes into a □Barrel Protein Host: Molecular-Docking and Reactivity Insights. *European Journal of Inorganic Chemistry*, **2017**, 2017, 3622-3634	2.2	7
46	Small Basis Set Allowing the Recovery of Dispersion Interactions with Double-Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2019**, 15, 2944-2953	6.4	7
45	Antagonistic Effect of Acetates in C□N Bond Formation with In Situ Generated Diazonium Salts: A Combined Theoretical and Experimental Study. *European Journal of Organic Chemistry*, **2016**, 2016, 5887-5896	2.2	7
44	Static and dynamic approaches for the calculation of NMR parameters: Permanganate ion as a case study. *Computational and Theoretical Chemistry*, **2006**, 762, 133-137		7
43	Electron Spin Densities and Density Functional Approximations: Open-Shell Polycyclic Aromatic Hydrocarbons as Case Study. *Journal of Chemical Theory and Computation*, **2020**, 16, 3567-3577	6.4	6
42	Spectral signature of a Ru(II, III, IV) complex: a combined experimental and theoretical investigation. *Dalton Transactions*, **2013**, 42, 7943-51	4.3	6
41	Theoretical investigation of the conformational behaviour of N-phenylbenzohydroxamic acid in solution. *Magnetic Resonance in Chemistry*, **2004**, 42 Spec no, S48-56	2.1	6
40	Ligand exchange on CdSe nanoplatelets for the solar light sensitization of TiO2 and ZnO nanorod arrays. *Journal of Photochemistry and Photobiology A: Chemistry*, **2019**, 368, 182-189	4.7	6
39	Evidence for a Cooperative Mechanism Involving Two Palladium(0) Centers in the Oxidative Addition of Iodoarenes. *Chemistry - A European Journal*, **2018**, 24, 2192-2199	4.8	6
38	A Comparative Investigation of the Role of the Anchoring Group on Perylene Monoimide Dyes in NiO-Based Dye-Sensitized Solar Cells. *ChemSusChem*, **2020**, 13, 1844-1855	8.3	6

37	Improving the heterointerface in hybrid organic-inorganic perovskite solar cells by surface engineering: Insights from periodic hybrid density functional theory calculations. *Journal of Computational Chemistry*, **2020**, 41, 1740-1747	3.5	5
36	Theoretical Study of Sticking Processes on Molecular Models of Silica Surfaces. *Theoretical Chemistry Accounts*, **2006**, 115, 379-384	1.9	5
35	Towards the modeling of quantum-dot sensitized solar cells: from structural and vibrational features to electron injection through lattice-mismatched interfaces. *Journal of Materials Chemistry A*, **2016**, 4, 13081-13092	13	4
34	Double-Hybrid Functionals and Tailored Basis Set: Fullerene (C) Dimer and Isomers as Test Cases. *Journal of Physical Chemistry A*, **2019**, 123, 10040-10046	2.8	4
33	In silico assessment of the HPLC□UV response coefficients. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 1-5	2	4
32	A DFT Protocol for the Prediction of 31P NMR Chemical Shifts of Phosphine Ligands in First-Row Transition-Metal Complexes. *Organometallics*, **2020**, 39, 3121-3130	3.8	4
31	Using density based indexes to characterize excited states evolution. *Journal of Computational Chemistry*, **2019**, 40, 650-656	3.5	4
30	Gradient-regulated connection-based correction for the PBE exchange: the PBEtrans model. *Molecular Physics*, **2016**, 114, 1059-1065	1.7	3
29	Pyrimidyl-substituted anthracene fluorophores: Syntheses, absorption spectra, and photophysical properties. *Dyes and Pigments*, **2018**, 159, 619-636	4.6	3
28	Photophysical properties of fluorescent imaging biological probes of nucleic acids: SAC-CI and TD-DFT Study. *Journal of Computational Chemistry*, **2019**, 40, 127-134	3.5	3
27	Ex situ and in situ sensitized quantum dot solar cells. *Physica Status Solidi (B): Basic Research*, **2017**, 254, 1600443	1.3	3
26	Simulations of UV□isible spectra for analytical applications: phenothiazines as a case study. *Molecular Simulation*, **2014**, 40, 169-175	2	3
25	Direct Synthesis of CFH-Substituted 2-Amidofurans via Copper-Catalyzed Addition of Difluorinated Diazoacetone to Ynamides. *Organic Letters*, **2021**, 23, 5528-5532	6.2	3
24	Toward a fast evaluation of g-tensor of Cu containing systems: A DFT parametrized approach. *Chemical Physics Letters*, **2014**, 614, 226-233	2.5	2
23	Toward blue emission in ZnO based LED **2012**,		2
22	Role of dppf Monoxide in the Transmetalation Step of the Suzuki□Miyaura Coupling Reaction. *Organometallics*, **2021**, 40, 1120-1128	3.8	2
21	Computation of covalent and noncovalent structural parameters at low computational cost: Efficiency of the DH-SVPD method. *International Journal of Quantum Chemistry*, **2020**, 120, e26233	2.1	2
20	Electronic coupling in the reduced state lies at the origin of color changes of ommochromes. *Dyes and Pigments*, **2021**, 185, 108661	4.6	2

19	Mechanochromic LLDPE Films Doped with NIR Reflective Paliogen Black. *Macromolecular Rapid Communications*, **2021**, 42, e2000426	4.8	2
18	Copper-catalyzed transformation of alkyl nitriles to -arylacetamide using diaryliodonium salts.. *RSC Advances*, **2021**, 11, 15885-15889	3.7	2
17	Following excited states in molecular systems using density-based indexes: A dual emissive system as a test case. *Journal of Photochemistry and Photobiology A: Chemistry*, **2019**, 383, 111978	4.7	1
16	Ruthenium(II) complexes with new large-surface ligands based on electron-accepting expanded pyridiniums: insights from density functional theory. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	1
15	Probing the performances of HISS functionals for the description of excited states of molecular systems. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	1
14	Chapter 14 Quantum chemical topology and reactivity: A comparative static and dynamic study on a SN2 reaction. *Theoretical and Computational Chemistry*, **2007**, 287-300		1
13	Silver(I) Oxide-/DBU-Promoted Synthesis of Dihydrofuran Units through Allenyl Silver Formation. *Chemistry - A European Journal*, **2020**, 26, 17455-17461	4.8	1
12	Chasing unphysical TD-DFT excited states in transition metal complexes with a simple diagnostic tool. *Journal of Chemical Physics*, **2021**, 154, 204102	3.9	1
11	Metal-Free Deoxygenation of Amine N-Oxides: Synthetic and Mechanistic Studies. *ChemPhysChem*, **2021**, 22, 1237-1242	3.2	1
10	Macrolactonization Reactions Driven by a Pentafluorobenzoyl Group*. *Angewandte Chemie - International Edition*, **2021**, 60, 19843-19851	16.4	1
9	A global analysis of excited states: the global transition contribution grids. *Theoretical Chemistry Accounts*, **2021**, 140, 1	1.9	0
8	Theoretical insights on acceptor-donor dyads for organic photovoltaics. *Physical Chemistry Chemical Physics*, **2020**, 22, 27413-27424	3.6	0
7	A combined Monte Carlo/DFT approach to simulate UV-vis spectra of molecules and aggregates: Merocyanine dyes as a case study. *Journal of Computational Chemistry*, **2021**, 42, 1054-1063	3.5	0
6	Modeling UV-Vis spectra of low dimensional materials using electrostatic embedding: The case of CdSe. *Journal of Computational Chemistry*, **2021**, 42, 1212-1224	3.5	0
5	Atypical Lone Pair□Interaction with Quinone Methides in a Series of Imido-Ferrociphenol Anticancer Drug Candidates. *Angewandte Chemie*, **2019**, 131, 8509	3.6	
4	Modeling the Electron Transfer Chain in an Artificial Photosynthetic Machine. *Journal of Physical Chemistry Letters*, **2020**, 11, 9738-9744	6.4	
3	On the Interplay between Molecular Packing and Optical Response in Thin Films for Organic Photovoltaics. *Journal of Physical Chemistry C*, **2021**, 125, 16304-16315	3.8	
2	Does the gradient-regulated connection improve the description of correlated metal bond properties?. *International Journal of Quantum Chemistry*, **2019**, 119, e25831	2.1	

1	Macrolactonization Reactions Driven by a Pentafluorobenzoyl Group**. *Angewandte Chemie*, **2021**, 133, 19996-20004	3.6