Carlo Adamo

List of Publications by Citations

443 papers	36,371 citations	78 h-index	181 g-index
468 ext. papers	39,840 ext. citations	4.4 avg, IF	7.67 L-index

#	Paper	IF	Citations
443	Toward reliable density functional methods without adjustable parameters: The PBE0 model. *Journal of Chemical Physics*, **1999**, 110, 6158-6170	3.9	11214
442	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	3.9	2722
441	The calculations of excited-state properties with Time-Dependent Density Functional Theory. *Chemical Society Reviews*, **2013**, 42, 845-56	58.5	1048
440	Extensive TD-DFT Benchmark: Singlet-Excited States of Organic Molecules. *Journal of Chemical Theory and Computation*, **2009**, 5, 2420-35	6.4	799
439	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
438	A Qualitative Index of Spatial Extent in Charge-Transfer Excitations. *Journal of Chemical Theory and Computation*, **2011**, 7, 2498-506	6.4	657
437	Toward reliable adiabatic connection models free from adjustable parameters. *Chemical Physics Letters*, **1997**, 274, 242-250	2.5	635
436	Accurate excitation energies from time-dependent density functional theory: Assessing the PBE0 model. *Journal of Chemical Physics*, **1999**, 111, 2889-2899	3.9	592
435	Accurate simulation of optical properties in dyes. *Accounts of Chemical Research*, **2009**, 42, 326-34	24.3	404
434	TD-DFT Assessment of Functionals for Optical 0-0 Transitions in Solvated Dyes. *Journal of Chemical Theory and Computation*, **2012**, 8, 2359-72	6.4	342
433	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
432	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
431	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	3.9	276
430	Assessment of the efficiency of long-range corrected functionals for some properties of large compounds. *Journal of Chemical Physics*, **2007**, 126, 144105	3.9	264
429	Excited-state calculations with TD-DFT: from benchmarks to simulations in complex environments. *Physical Chemistry Chemical Physics*, **2011**, 13, 16987-98	3.6	258
428	On the Metric of Charge Transfer Molecular Excitations: A Simple Chemical Descriptor. *Journal of Chemical Theory and Computation*, **2013**, 9, 3118-26	6.4	247
427	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

426	Toward chemical accuracy in the computation of NMR shieldings: the PBE0 model. *Chemical Physics Letters*, **1998**, 298, 113-119	2.5	226
425	Dye chemistry with time-dependent density functional theory. *Physical Chemistry Chemical Physics*, **2014**, 16, 14334-56	3.6	225
424	Proton transfer in the ground and lowest excited states of malonaldehyde: A comparative density functional and post-Hartree□Fock study. *Journal of Chemical Physics*, **1996**, 105, 11007-11019	3.9	201
423	Choosing a Functional for Computing Absorption and Fluorescence Band Shapes with TD-DFT. *Journal of Chemical Theory and Computation*, **2013**, 9, 2749-60	6.4	196
422	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
421	Through-Space Charge Transfer in Rod-Like Molecules: Lessons from Theory. *Journal of Physical Chemistry C*, **2012**, 116, 11946-11955	3.8	193
420	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	2.5	186
419	First-principles modeling of dye-sensitized solar cells: challenges and perspectives. *Accounts of Chemical Research*, **2012**, 45, 1268-77	24.3	182
418	Structural and Electronic Properties of Selected Rutile and Anatase TiO2 Surfaces: An ab Initio Investigation. *Journal of Chemical Theory and Computation*, **2008**, 4, 341-52	6.4	182
417	Assessment of Functionals for TD-DFT Calculations of Singlet-Triplet Transitions. *Journal of Chemical Theory and Computation*, **2010**, 6, 1532-7	6.4	173
416	Seeking for parameter-free double-hybrid functionals: the PBE0-DH model. *Journal of Chemical Physics*, **2011**, 135, 024106	3.9	171
415	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	2.8	166
414	Predicting proton transfer barriers with density functional methods. *Chemical Physics Letters*, **1999**, 306, 83-87	2.5	164
413	Conformational behavior of gaseous glycine by a density functional approach. *Journal of Chemical Physics*, **1995**, 102, 364-370	3.9	162
412	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
411	First hyperpolarizability of polymethineimine with long-range corrected functionals. *Journal of Chemical Physics*, **2007**, 126, 191108	3.9	151
410	An accurate density functional method for the study of magnetic properties: the PBE0 model. *Computational and Theoretical Chemistry*, **1999**, 493, 145-157		147
409	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

408	Validation of self-consistent hybrid density functionals for the study of structural and electronic characteristics of organic radicals. *Journal of Chemical Physics*, **1995**, 102, 384-393	3.9	133
407	Inexpensive and accurate predictions of optical excitations in transition-metal complexes: the TDDFT/PBE0 route. *Theoretical Chemistry Accounts*, **2000**, 105, 169-172	1.9	126
406	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
405	Bond Length Alternation of Conjugated Oligomers: Wave Function and DFT Benchmarks. *Journal of Chemical Theory and Computation*, **2011**, 7, 369-76	6.4	119
404	Physically motivated density functionals with improved performances: The modified PerdewBurkeErnzerhof model. *Journal of Chemical Physics*, **2002**, 116, 5933-5940	3.9	119
403	Assessment of the B97 family for excited-state calculations. *Theoretical Chemistry Accounts*, **2011**, 128, 127-136	1.9	115
402	Performance of an Optimally Tuned Range-Separated Hybrid Functional for 0-0 Electronic Excitation Energies. *Journal of Chemical Theory and Computation*, **2014**, 10, 1677-85	6.4	113
401	Planar vs. twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory. *Physical Chemistry Chemical Physics*, **2010**, 12, 8016-23	3.6	113
400	Assessment of long-range corrected functionals performance for n-->pi* transitions in organic dyes. *Journal of Chemical Physics*, **2007**, 127, 094102	3.9	112
399	Benchmarking Density Functionals on Structural Parameters of Small-/Medium-Sized Organic Molecules. *Journal of Chemical Theory and Computation*, **2016**, 12, 459-65	6.4	110
398	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
397	Communication: double-hybrid functionals from adiabatic-connection: the QIDH model. *Journal of Chemical Physics*, **2014**, 141, 031101	3.9	108
396	Accurate excitation energies from time-dependent density functional theory: assessing the PBE0 model for organic free radicals. *Chemical Physics Letters*, **1999**, 314, 152-157	2.5	106
395	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
394	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
393	Spectroscopic properties of porphyrin-like photosensitizers: insights from theory. *Journal of Physical Chemistry B*, **2006**, 110, 2398-404	3.4	104
392	Contribution to the Mechanism of Copper-Catalyzed CN and CO Bond Formation. *Organometallics*, **2012**, 31, 7694-7707	3.8	101
391	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

390	A hybrid density functional study of the first-row transition-metal monocarbonyls. *Journal of Chemical Physics*, **1995**, 103, 10605-10613	3.9	96
389	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, 5782-90	6.4	95
388	Comment on "about the calculation of exchange coupling constants using density-functional theory: the role of the self-interaction error" [J. Chem. Phys. 123, 164110 (2005)]. *Journal of Chemical Physics*, **2006**, 124, 107101; author reply 107102	3.9	95
387	Exploring excited states using Time Dependent Density Functional Theory and density-based indexes. *Coordination Chemistry Reviews*, **2015**, 304-305, 166-178	23.2	94
386	Phototriggered Linkage Isomerization in RutheniumDimethylsulfoxyde Complexes:Insights from Theory. *Journal of Physical Chemistry A*, **2003**, 107, 11182-11190	2.8	94
385	Density Functional Study of Intrinsic and Environmental Effects in the Tautomeric Equilibrium of 2-Pyridone. *The Journal of Physical Chemistry*, **1995**, 99, 15062-15068		94
384	Surface-dependent oxidation of H 2 on CeO 2 surfaces. *Journal of Catalysis*, **2013**, 297, 193-201	7.3	93
383	Modeling Dye-Sensitized Solar Cells: From Theory to Experiment. *Journal of Physical Chemistry Letters*, **2013**, 4, 1044-50	6.4	93
382	The meta-GGA functional: Thermochemistry with a kinetic energy density dependent exchange-correlation functional. *Journal of Chemical Physics*, **2000**, 112, 2643-2649	3.9	93
381	A Theoretical Study of Bonding in Lanthanide Trihalides by Density Functional Methods. *Journal of Physical Chemistry A*, **1998**, 102, 6812-6820	2.8	90
380	Proton transfer in model hydrogen-bonded systems by a density functional approach. *Chemical Physics Letters*, **1994**, 231, 295-300	2.5	90
379	Extensive TD-DFT investigation of the first electronic transition in substituted azobenzenes. *Chemical Physics Letters*, **2008**, 465, 226-229	2.5	88
378	A General Guidebook for the Theoretical Prediction of Physicochemical Properties of Chemicals for Regulatory Purposes. *Chemical Reviews*, **2015**, 115, 13093-164	68.1	87
377	Orthorhombic BiFeO3. *Physical Review Letters*, **2012**, 109, 247606	7.4	87
376	Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. *Journal of Chemical Physics*, **2012**, 136, 174103	3.9	86
375	Performance of the 'parameter free' PBE0 functional for the modeling of molecular properties of heavy metals. *Chemical Physics Letters*, **2000**, 325, 99-105	2.5	86
374	Communication: one third: a new recipe for the PBE0 paradigm. *Journal of Chemical Physics*, **2013**, 138, 021104	3.9	84
373	Communication: rationale for a new class of double-hybrid approximations in density-functional theory. *Journal of Chemical Physics*, **2011**, 135, 101102	3.9	83

372	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	3.5	83
371	Comparative studies of quasi-relativistic density functional methods for the description of lanthanide and actinide complexes. *Journal of Computational Chemistry*, **2003**, 24, 850-8	3.5	82
370	Accurate static polarizabilities by density functional theory: assessment of the PBE0 model. *Chemical Physics Letters*, **1999**, 307, 265-271	2.5	82
369	Localized excited charge carriers generate ultrafast inhomogeneous strain in the multiferroic BiFeO3. *Physical Review Letters*, **2014**, 112, 097602	7.4	80
368	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	2.5	80
367	Double-hybrid density functionals: merging wavefunction and density approaches to get the best of both worlds. *Physical Chemistry Chemical Physics*, **2013**, 15, 14581-94	3.6	79
366	Validation and assessment of an accurate approach to the correlation problem in density functional theory: The Krieger□Chen□afrate□avin model. *Journal of Chemical Physics*, **2002**, 117, 10465-10473	3.9	79
365	Is the Tamm-Dancoff Approximation Reliable for the Calculation of Absorption and Fluorescence Band Shapes?. *Journal of Chemical Theory and Computation*, **2013**, 9, 4517-25	6.4	75
364	Nonempirical Double-Hybrid Functionals: An Effective Tool for Chemists. *Accounts of Chemical Research*, **2016**, 49, 1503-13	24.3	75
363	Absorption spectra of first-row transition metal complexes of bacteriochlorins: a theoretical analysis. *Journal of Physical Chemistry B*, **2005**, 109, 12214-21	3.4	74
362	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
361	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
360	DFT and Proton Transfer Reactions: A Benchmark Study on Structure and Kinetics. *Journal of Chemical Theory and Computation*, **2012**, 8, 3082-8	6.4	69
359	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, 13402-10	2.8	69
358	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. *Inorganic Chemistry*, **2006**, 45, 8517-22	5.1	69
357	A comprehensive theoretical view of the bonding in actinide molecular complexes. *Journal of the American Chemical Society*, **2006**, 128, 2190-1	16.4	69
356	Theoretical Unraveling of Selective 1-Butene Oligomerization Catalyzed by Iron□is(arylimino)pyridine. *Organometallics*, **2009**, 28, 5358-5367	3.8	68
355	Predictions of Optical Excitations in Transition-Metal Complexes with Time Dependent-Density Functional Theory: Influence of Basis Sets. *Journal of Chemical Theory and Computation*, **2005**, 1, 953-62	6.4	67

354	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
353	Oxidation mechanism of diethyl ether: a complex process for a simple molecule. *Physical Chemistry Chemical Physics*, **2011**, 13, 14636-45	3.6	64
352	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
351	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
350	Functionalized Graphene as an Electron-Cascade Acceptor for Air-Processed Organic Ternary Solar Cells. *Advanced Functional Materials*, **2015**, 25, 3870-3880	15.6	63
349	Ionic versus covalent character in lanthanide complexes. A hybrid density functional study. *Chemical Physics Letters*, **1997**, 268, 61-68	2.5	62
348	First-row transition-metal hydrides: A challenging playground for new theoretical approaches. *International Journal of Quantum Chemistry*, **1997**, 61, 443-451	2.1	60
347	The geometries, absorption and fluorescence wavelengths of solvated fluorescent coumarins: A CIS and TD-DFT comparative study. *Chemical Physics Letters*, **2007**, 438, 208-212	2.5	60
346	Ab Initio Molecular Dynamics Study of a Highly Concentrated LiCl Aqueous Solution. *Journal of Chemical Theory and Computation*, **2008**, 4, 1040-8	6.4	59
345	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	16.4	59
344	Spectral properties of self-assembled squaraine-tetralactam: a theoretical assessment. *Physical Chemistry Chemical Physics*, **2009**, 11, 1258-62	3.6	57
343	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
342	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
341	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
340	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	2.5	54
339	Evaluating push-pull dye efficiency using TD-DFT and charge transfer indices. *Physical Chemistry Chemical Physics*, **2013**, 15, 20210-9	3.6	53
338	Absorption and emission spectra of 1,8-naphthalimide fluorophores: A PCM-TD-DFT investigation. *Chemical Physics*, **2010**, 372, 61-66	2.3	53
337	Structure and magnetic properties of benzyl, anilino, and phenoxyl radicals by density functional computations. *Journal of Chemical Physics*, **1998**, 109, 10244-10254	3.9	53

336	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
335	Effective electron displacements: a tool for time-dependent density functional theory computational spectroscopy. *Journal of Chemical Physics*, **2014**, 140, 104101	3.9	50
334	Exploring the metric of excited state proton transfer reactions. *Journal of Physical Chemistry B*, **2013**, 117, 16165-73	3.4	50
333	On the TD-DFT UV/vis spectra accuracy: the azoalkanes. *Theoretical Chemistry Accounts*, **2008**, 120, 405-410	1.9	50
332	A comprehensive DFT investigation of bulk and low-index surfaces of ZrO2 polymorphs. *Journal of Computational Chemistry*, **2015**, 36, 9-21	3.5	49
331	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	13.1	49
330	A new parameter-free correlation functional based on an average atomic reduced density gradient analysis. *Journal of Chemical Physics*, **2008**, 128, 034101	3.9	49
329	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
328	From Classical Density Functionals to Adiabatic Connection Methods. The State of the Art.. *Advances in Quantum Chemistry*, **2000**, 36, 45-75	1.4	48
327	Transport properties in manganite thin films. *Physical Review B*, **2005**, 71,	3.3	47
326	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
325	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
324	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
323	Modeling ZnO phases using a periodic approach: from bulk to surface and beyond. *Journal of Chemical Physics*, **2009**, 131, 044708	3.9	43
322	Solvent effects on an SN2 reaction profile. *Chemical Physics Letters*, **1998**, 297, 1-7	2.5	43
321	Theoretical study of the decomposition reactions in substituted nitrobenzenes. *Journal of Physical Chemistry A*, **2008**, 112, 4054-9	2.8	43
320	Phosphorescent binuclear iridium complexes based on terpyridine-carboxylate: an experimental and theoretical study. *Inorganic Chemistry*, **2011**, 50, 8197-206	5.1	42
319	Catalytic and bulk solvent effects on proton transfer: Formamide as a case study. *Journal of Computational Chemistry*, **1997**, 18, 1993-2000	3.5	42

318	Intramolecular spin alignment in photomagnetic molecular devices: a theoretical study. *Chemistry - A European Journal*, **2007**, 13, 5360-77	4.8	42
317	Density Functional Study of Diborane, Dialane, and Digallane. *The Journal of Physical Chemistry*, **1994**, 98, 13185-13188		42
316	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
315	Range-separated hybrid density functionals made simple. *Journal of Chemical Physics*, **2019**, 150, 201102	3.9	40
314	Theoretical Exploration of Type I/Type II Dual Photoreactivity of Promising Ru(II) Dyads for PDT Approach. *Inorganic Chemistry*, **2016**, 55, 11185-11192	5.1	40
313	Accuracy of TD-DFT Geometries: A Fresh Look. *Journal of Chemical Theory and Computation*, **2018**, 14, 3715-3727	6.4	40
312	Fluorescence of 1,8-naphthalimide: A PCM-TD-DFT investigation. *Chemical Physics Letters*, **2007**, 448, 3-6	2.5	40
311	Bi-isonicotinic Acid on Anatase (101): Insights from Theory. *Journal of Physical Chemistry C*, **2007**, 111, 15034-15042	3.8	40
310	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	2.5	40
309	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
308	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
307	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
306	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	3.9	38
305	Structure and ESR features of glycine radical in its zwitterionic form. *Chemical Physics Letters*, **1995**, 242, 351-354	2.5	38
304	Understanding Aggregation-Induced Emission in Molecular Crystals: Insights from Theory. *Journal of Physical Chemistry C*, **2017**, 121, 5747-5752	3.8	37
303	Theoretical Investigation of Hole Transporter Materials for Energy Devices. *Journal of Physical Chemistry C*, **2015**, 119, 23890-23898	3.8	37
302	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
301	Characterizing agosticity using the quantum theory of atoms in molecules: bond critical points and their local properties. *Journal of Physical Chemistry A*, **2012**, 116, 5472-9	2.8	37

300	A theoretical study of the decomposition mechanisms in substituted o-nitrotoluenes. *Journal of Physical Chemistry A*, **2009**, 113, 13621-7	2.8	37
299	CO Oxidation on Cationic Gold Clusters: A Theoretical Study. *Journal of Physical Chemistry C*, **2008**, 112, 18061-18066	3.8	37
298	Electronic Band Shapes Calculated with Optimally Tuned Range-Separated Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 4599-608	6.4	36
297	Non-radiative decay paths in rhodamines: new theoretical insights. *Physical Chemistry Chemical Physics*, **2014**, 16, 20681-8	3.6	35
296	Basis set and functional effects on excited-state properties: Three bicyclic chromogens as working examples. *International Journal of Quantum Chemistry*, **2012**, 112, 2135-2141	2.1	35
295	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, 10849-58	3.6	35
294	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
293	Evidence for the Iron(III) Oxidation State in Bis(imino)pyridine Catalysts. A Density Functional Theory Study. *Organometallics*, **2008**, 27, 3368-3377	3.8	35
292	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	3.5	35
291	Systematic Improvement of Density Functionals through Parameter-Free Hybridization Schemes. *Journal of Physical Chemistry Letters*, **2015**, 6, 3540-5	6.4	34
290	On the prediction of thermal stability of nitroaromatic compounds using quantum chemical calculations. *Journal of Hazardous Materials*, **2009**, 171, 845-50	12.8	34
289	Tuning of Structural and Magnetic Properties of Nitronyl Nitroxides by the Environment. A Combined Experimental and Computational Study. *Journal of Physical Chemistry A*, **1999**, 103, 3481-3488	2.8	34
288	Structure and ESR Features of Glycine Radical. *Journal of the American Chemical Society*, **1995**, 117, 12618-12624	14.4	34
287	Density functional theory: An effective theoretical tool for the study of radicals. *International Journal of Quantum Chemistry*, **1994**, 52, 963-971	2.1	34
286	Intermolecular proton shuttling in excited state proton transfer reactions: insights from theory. *Physical Chemistry Chemical Physics*, **2014**, 16, 8661-6	3.6	33
285	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
284	B,N-Codoped graphene as catalyst for the oxygen reduction reaction: Insights from periodic and cluster DFT calculations. *Journal of Computational Chemistry*, **2018**, 39, 637-647	3.5	32
283	Range-Separated Double-Hybrid Functional from Nonempirical Constraints. *Journal of Chemical Theory and Computation*, **2018**, 14, 4052-4062	6.4	32

282	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
281	Discriminating role of bases in diketonate copper(I)-catalyzed C-O couplings: phenol versus diarylether. *Dalton Transactions*, **2013**, 42, 5348-54	4.3	32
280	Absorption spectra of azobenzenes simulated with time-dependent density functional theory. *International Journal of Quantum Chemistry*, **2011**, 111, 4224-4240	2.1	32
279	Validation of Hybrid Density Functional/Hartree□Fock Approaches for the Study of Homogeneous Catalysis. *The Journal of Physical Chemistry*, **1996**, 100, 2094-2099		32
278	Fast and reliable theoretical determination of pKa* for photoacids. *Journal of Physical Chemistry A*, **2008**, 112, 794-6	2.8	32
277	Pd-catalyzed homocoupling reaction of arylboronic acid: insights from density functional theory. *Journal of Physical Chemistry A*, **2008**, 112, 12896-903	2.8	32
276	Intrinsic and environmental effects in the physico-chemical properties of nitroxides. The case of 2-phenyl-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazol-1-oxyl 3-oxide. *Chemical Physics Letters*, **1999**, 310, 159-165	2.5	32
275	Oxidation of Ethylbenzene to Acetophenone with N-Doped Graphene: Insight from Theory. *Journal of Physical Chemistry C*, **2014**, 118, 12275-12284	3.8	31
274	A reliable method for fitting TD-DFT transitions to experimental UV□isible spectra. *Computational and Theoretical Chemistry*, **2010**, 954, 52-56		31
273	Theoretical analysis of the electronic properties of N3 derivatives. *Journal of Physical Chemistry A*, **2007**, 111, 13106-11	2.8	31
272	DFT modeling of the relative affinity of nitrogen ligands for trivalent f elements: an energetic point of view. *New Journal of Chemistry*, **2007**, 31, 1738	3.6	31
271	Increasing physical constraints and improving performances in a parameter-free GGA functional. *Chemical Physics Letters*, **2008**, 460, 536-539	2.5	31
270	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
269	Hydrogen abstraction from ethylbenzene by imide-N-oxyl radicals with and without O2: a DFT theoretical study. *Perkin Transactions II RSC*, **2002**, 1967-1972		31
268	Charge transfer excitations in TDDFT: A ghost-hunter index. *Journal of Computational Chemistry*, **2017**, 38, 2151-2156	3.5	30
267	Intrinsic and dynamical reaction pathways of an excited state proton transfer. *Journal of Physical Chemistry B*, **2015**, 119, 2650-7	3.4	30
266	A comparison of geometric parameters from PBE-based doubly hybrid density functionals PBE0-DH, PBE0-2, and xDH-PBE0. *Journal of Chemical Physics*, **2013**, 139, 174106	3.9	30
265	On the use of descriptors arising from the conceptual density functional theory for the prediction of chemicals explosibility. *Chemical Physics Letters*, **2009**, 467, 407-411	2.5	30

264	Toward a combined DFT/QTAIM description of agostic bonds: the critical case of a Nb(III) complex. *Journal of Physical Chemistry A*, **2009**, 113, 12322-7	2.8	30
263	Vibrational analysis of glycine radical: a comparative ab initio static and dynamic study. *Physical Chemistry Chemical Physics*, **2009**, 11, 4375-84	3.6	30
262	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
261	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*, **2018**, 21, 46-56	3.6	29
260	Importance of Orbital Optimization for Double-Hybrid Density Functionals: Application of the OO-PBE-QIDH Model for Closed- and Open-Shell Systems. *Journal of Physical Chemistry A*, **2016**, 120, 1756-62	2.8	29
259	Photophysical properties of NIR-emitting fluorescence probes: insights from TD-DFT. *Physical Chemistry Chemical Physics*, **2013**, 15, 10019-27	3.6	29
258	Development of a QSPR model for predicting thermal stabilities of nitroaromatic compounds taking into account their decomposition mechanisms. *Journal of Molecular Modeling*, **2011**, 17, 2443-53	2	29
257	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
256	Conformational Behavior and Magnetic Properties of Organic Radicals Derived from Amino Acid Residues. The Dipeptide Analog of Glycine Radical. *Journal of the American Chemical Society*, **1995**, 117, 1083-1089	16.4	29
255	Density Functional Calculations of Isotropic Hyperfine Coupling Constants in .beta.-Ketoenolyl Radicals. *The Journal of Physical Chemistry*, **1994**, 98, 8648-8652		29
254	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
253	Low temperature magnetism in the perovskite substrate DyScO3. *Applied Physics Letters*, **2009**, 94, 152503	3.4	28
252	A theoretical characterization of covalency in rare earth complexes through their absorption electronic properties: f-f transitions. *Inorganic Chemistry*, **2006**, 45, 7382-8	5.1	28
251	A theoretical investigation of potential energy surfaces governing the photochemical tautomerization of 2-pyridone. *Chemical Physics Letters*, **1994**, 226, 399-404	2.5	28
250	Quadratic integrand double-hybrid made spin-component-scaled. *Journal of Chemical Physics*, **2016**, 144, 124104	3.9	27
249	Modeling basic components of solid oxide fuel cells using density functional theory: Bulk and surface properties of CeO2. *Surface Science*, **2012**, 606, 305-311	1.8	27
248	Theoretical insights on the electronic properties of eosin Y, an organic dye for photovoltaic applications. *Journal of Physical Chemistry A*, **2008**, 112, 7264-70	2.8	27
247	Reaching optimal light-induced intramolecular spin alignment within photomagnetic molecular device prototypes. *Chemistry - A European Journal*, **2008**, 14, 11385-405	4.8	27

246	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
245	A theoretical study of proton transfer in [2,2?-bipyridyl]-3,3?-diol. *Chemical Physics Letters*, **1995**, 241, 1-6	2.5	27
244	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
243	Prediction of the thermal decomposition of organic peroxides by validated QSPR models. *Journal of Hazardous Materials*, **2014**, 276, 216-24	12.8	26
242	Charge transport in poly-imidazole membranes: a fresh appraisal of the Grotthuss mechanism. *Physical Chemistry Chemical Physics*, **2012**, 14, 10910-8	3.6	26
241	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
240	A DFT investigation of CO oxidation over neutral and cationic gold clusters. *Computational and Theoretical Chemistry*, **2009**, 903, 34-40		26
239	QSPR modeling of thermal stability of nitroaromatic compounds: DFT vs. AM1 calculated descriptors. *Journal of Molecular Modeling*, **2010**, 16, 805-12	2	26
238	Theoretical description of metal□ligand bonding within f-element complexes: A successful and necessary interplay between theory and experiment. *Comptes Rendus Chimie*, **2007**, 10, 888-896	2.7	26
237	Solvent effects on the conformational behavior of model peptides. A comparison between different continuum models. *Chemical Physics Letters*, **1996**, 263, 113-118	2.5	26
236	Speed-Up of the Excited-State Benchmarking: Double-Hybrid Density Functionals as Test Cases. *Journal of Chemical Theory and Computation*, **2017**, 13, 5539-5551	6.4	25
235	Computational Molecular Electronic Spectroscopy with TD-DFT. *Topics in Current Chemistry*, **2016**, 368, 347-75		25
234	Performance of a new hybrid Hartree□Fock/Kohn□Sham model (B98) in predicting vibrational frequencies, polarisabilities and NMR chemical shifts. *Chemical Physics Letters*, **1999**, 311, 69-76	2.5	25
233	Proton transfer in small model systems: A density functional study. *International Journal of Quantum Chemistry*, **1995**, 56, 697-705	2.1	25
232	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
231	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
230	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
229	Ammonia on Ni(111) surface studied by first principles: Bonding, multilayers structure and comparison with experimental IR and XPS data. *Surface Science*, **2009**, 603, 3025-3034	1.8	24

228	Room temperature metal-insulator transition in as grown (La (mathsf{_{1-x}})Sr(mathsf{_{x}}))(mathsf{_{y}})MnO(mathsf{_{3}}) thin films deposited by molecular beam epitaxy. *European Physical Journal B*, **2004**, 40, 11-17	1.2	24
227	A new hybrid functional including a meta-GGA approach. *Chemical Physics Letters*, **2002**, 362, 72-78	2.5	24
226	Role of Hartree-Fock exchange in density functional theory. *Chemical Physics Letters*, **1994**, 230, 189-195	2.5	24
225	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
224	Modeling proton transfer in imidazole-like dimers: a density functional theory study. *Journal of Physical Chemistry A*, **2011**, 115, 2627-34	2.8	23
223	Absorption spectra of recently synthesised organic dyes: A TD-DFT study. *International Journal of Quantum Chemistry*, **2010**, 110, 2121-2129	2.1	23
222	Toward a general protocol for the study of static and dynamic properties of hydrogen-bonded systems. *International Journal of Quantum Chemistry*, **1997**, 61, 429-442	2.1	23
221	Comparative Static and Dynamic Study of a Prototype SN2 Reaction. *Journal of Chemical Theory and Computation*, **2006**, 2, 1220-7	6.4	23
220	A theoretical study of the bonding in trivalent americium complexes. *Chemical Physics Letters*, **2004**, 396, 452-457	2.5	23
219	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
218	Synergistic Effects of Metals in a Promising Ru(II) -Pt(II) Assembly for a Combined Anticancer Approach: Theoretical Exploration of the Photophysical Properties. *Chemistry - A European Journal*, **2016**, 22, 9162-8	4.8	23
217	La0.7Sr0.3MnO3 suspended microbridges for uncooled bolometers made using reactive ion etching of the silicon substrates. *Microelectronic Engineering*, **2013**, 111, 101-104	2.5	22
216	Revisiting the importance of dye binding mode in dye-sensitized solar cells: a periodic viewpoint. *Journal of Materials Chemistry*, **2012**, 22, 12205		22
215	Confinement Effects on UV-Visible Absorption Spectra: □Carotene Inside Carbon Nanotube as a Test Case. *Journal of Physical Chemistry Letters*, **2013**, 4, 1239-43	6.4	22
214	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
213	Excited-state properties from ground-state DFT descriptors: A QSPR approach for dyes. *Journal of Molecular Graphics and Modelling*, **2010**, 28, 465-71	2.8	22
212	Revisiting the nonlinear optical properties of polybutatriene and polydiacetylene with density functional theory. *Chemical Physics Letters*, **2008**, 456, 101-104	2.5	22
211	Density-functional-based molecular-dynamics simulations of molten salts. *Journal of Chemical Physics*, **2005**, 123, 134510	3.9	22

210	Interplay of intrinsic and environmental effects on the magnetic properties of free radicals issuing from H-atom addition to cytosine. *Journal of the American Chemical Society*, **2001**, 123, 7113-7	16.4	22
209	sp-hybridized carbon allotrope molecular structures: An ongoing challenge for density-functional approximations. *Journal of Chemical Physics*, **2019**, 151, 211104	3.9	22
208	Development of validated QSPR models for impact sensitivity of nitroaliphatic compounds. *Journal of Hazardous Materials*, **2012**, 235-236, 169-77	12.8	21
207	Predicting the Thermal Stability of Nitroaromatic Compounds Using Chemoinformatic Tools. *Molecular Informatics*, **2011**, 30, 623-34	3.8	21
206	Molecular dynamics study of the coordination sphere of trivalent lanthanum in a highly concentrated LiCl aqueous solution: a combined classical and ab initio approach. *Journal of Physical Chemistry B*, **2008**, 112, 10603-7	3.4	21
205	Spectral properties of bipyridyl ligands by time-dependent density functional theory. *Chemical Physics Letters*, **2006**, 417, 445-451	2.5	21
204	Direct catalytic effect and fine modulation of solvent in the keto-enol isomerization of amides. *Computational and Theoretical Chemistry*, **1995**, 330, 325-333		21
203	Modeling emission features of salicylidene aniline molecular crystals: A QM/QM' approach. *Journal of Computational Chemistry*, **2016**, 37, 861-70	3.5	21
202	Exploring the limits of recent exchange□correlation functionals in modeling lithium/benzene interaction. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	20
201	Theoretical study of the uranyl complexation by hydroxamic and carboxylic acid groups. *Inorganic Chemistry*, **2008**, 47, 7983-91	5.1	20
200	Structures, hyperfine parameters, and inversion barriers of cyclopropyl and oxiranyl radicals. *Journal of Chemical Physics*, **1996**, 105, 3168-3174	3.9	20
199	Equilibrium solvent effect in the framework of density functional theory. Application to the study of the thermodynamics of some organic and inorganic tautomeric equilibria. *Chemical Physics Letters*, **1994**, 223, 54-60	2.5	20
198	Double hybrid functionals and the □system bond length alternation challenge: rivaling accuracy of post-HF methods. *Journal of Chemical Theory and Computation*, **2015**, 11, 832-8	6.4	19
197	Revealing the properties of the cubic ZrO2 (111) surface by periodic DFT calculations: reducibility and stabilization through doping with aliovalent Y2O3. *RSC Advances*, **2015**, 5, 13941-13951	3.7	19
196	Communication: Bond length alternation of conjugated oligomers: Another step on the fifth rung of Perdew's ladder of functional. *Journal of Chemical Physics*, **2010**, 133, 151104	3.9	19
195	The performances of a parameter-free local correlation functional: The Ragot□ortona model. *Chemical Physics Letters*, **2007**, 439, 381-385	2.5	19
194	Comparison of theoretical approaches for computing the bond length alternation of polymethineimine. *Chemical Physics*, **2007**, 332, 79-85	2.3	19
193	The mechanism of spin polarization in aromatic free radicals. *Theoretical Chemistry Accounts*, **2000**, 104, 207-209	1.9	19

192	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
191	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
190	Computational Insights into Excited-State Proton-Transfer Reactions in Azo and Azomethine Dyes. *ChemPhysChem*, **2015**, 16, 3966-73	3.2	18
189	A combined experimental and theoretical study on the conformational behavior of a calix[6]arene. *Journal of Physical Chemistry A*, **2006**, 110, 5782-91	2.8	18
188	Solvation effects on cation interactions: a test study involving the quaternary ammonium ion. *Theoretical Chemistry Accounts*, **2004**, 111, 176-181	1.9	18
187	Protomeric equilibria in the ground and excited states of 2-pyridone. A semiempirical study including solvent effects. *Journal of the Chemical Society Perkin Transactions II*, **1993**, 697		18
186	Structure and EPR parameters of CuC2H2 from a density functional approach. *Chemical Physics Letters*, **1995**, 237, 189-194	2.5	18
185	A theoretical analysis of excited state proton transfer in 3-hydroxyflavone. Promoting effect of a low frequency bending mode. *Journal of Mathematical Chemistry*, **1992**, 10, 249-274	2.1	18
184	Benchmarking the DFT methodology for assessing antioxidant-related properties: quercetin and edaravone as case studies. *Journal of Molecular Modeling*, **2016**, 22, 250	2	18
183	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
182	Computational study of alkynes insertion into metal-hydride bonds catalyzed by bimetallic complexes. *Inorganic Chemistry*, **2010**, 49, 9875-83	5.1	17
181	A density functional study of bonding of water to copper and nickel atoms. *Computational and Theoretical Chemistry*, **1997**, 389, 83-89		17
180	Mapping the many-electron generalised spin-exchange Hamiltonian to accurate post-HF calculations. *Chemical Physics*, **2005**, 309, 133-141	2.3	17
179	Theoretical Study of a New Building Block for Organic Conductors: Tetrathiapentalene and Its Radical Cation. *Journal of Physical Chemistry B*, **1999**, 103, 6863-6869	3.4	17
178	Partnering dispersion corrections with modern parameter-free double-hybrid density functionals. *Physical Chemistry Chemical Physics*, **2017**, 19, 13481-13487	3.6	16
177	Non-parametrized functionals with empirical dispersion corrections: A happy match?. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	16
176	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
175	Conduction Mechanisms in Oxide Carbonate Electrolytes for SOFC: Highlighting the Role of the Interface from First-Principles Modeling. *Journal of Physical Chemistry C*, **2018**, 122, 10067-10077	3.8	16

174	Anchoring groups for dyes in p-DSSC application: insights from DFT. *Journal of Molecular Modeling*, **2016**, 22, 289	2	16
173	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
172	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
171	Role of nonlocal exchange in molecular crystals: the case of two proton-ordered phases of ice. *Journal of Computational Chemistry*, **2011**, 32, 2177-85	3.5	16
170	Predicting explosibility properties of chemicals from quantitative structure-property relationships. *Process Safety Progress*, **2010**, 29, 359-371	1	16
169	Modulation of intramolecular proton transfer by electronic excitation and environment: 2-Pyridone as a case study. *Journal of Computational Chemistry*, **1994**, 15, 395-404	3.5	16
168	Unveiling the Reactivity of a Synthetic Mimic of the Oxygen Evolving Complex. *Journal of Physical Chemistry Letters*, **2016**, 7, 5015-5021	6.4	15
167	Modeling the photosensitizing properties of thiolate-protected gold nanoclusters. *Physical Chemistry Chemical Physics*, **2016**, 18, 7737-50	3.6	15
166	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
165	Activation enthalpies of pericyclic reactions: the performances of some recently proposed functionals. *Theoretical Chemistry Accounts*, **2009**, 122, 257-264	1.9	15
164	Interconfigurational energies and ionization potentials: Test of a correlation energy functional. *Chemical Physics*, **2007**, 337, 161-167	2.3	15
163	Theoretical modelling of photoactive molecular systems: insights using the Density Functional Theory. *Comptes Rendus Chimie*, **2006**, 9, 226-239	2.7	15
162	New computational strategies for the quantum mechanical study of biological systems in condensed phases. *Theoretical and Computational Chemistry*, **2001**, 467-538		15
161	Towards an effective computational tool for the study of radiation-induced lesions of DNA bases. *Chemical Physics Letters*, **1999**, 301, 255-262	2.5	15
160	Transition metal monocarbonyls in the first excited electronic state. A hybrid density functional study. *Chemical Physics Letters*, **1995**, 246, 463-468	2.5	15
159	Copper-amyloid- complex may catalyze peroxynitrite production in brain: evidence from molecular modeling. *Physical Chemistry Chemical Physics*, **2014**, 16, 10169-74	3.6	14
158	On the development of QSPR models for regulatory frameworks: The heat of decomposition of nitroaromatics as a test case. *Journal of Loss Prevention in the Process Industries*, **2013**, 26, 1100-1105	3.5	14
157	Synergistic Effects in Pt -Porphyrinoid Dyes as Candidates for a Dual-Action Anticancer Therapy: A Theoretical Exploration. *Chemistry - A European Journal*, **2017**, 23, 15124-15132	4.8	14

156	Global and local quantitative structure–property relationship models to predict the impact sensitivity of nitro compounds. *Process Safety Progress*, **2012**, 31, 291-303	1	14
155	Communications: Making density functional theory and the quantum theory of atoms in molecules converse: a local approach. *Journal of Chemical Physics*, **2010**, 132, 211101	3.9	14
154	A density functional theory study of uranium(VI) nitrate monoamide complexes. *Physical Chemistry Chemical Physics*, **2011**, 13, 19371-7	3.6	14
153	Spin trapping by bis(benzene)chromium: A density functional study. *Physical Chemistry Chemical Physics*, **2003**, 5, 1337	3.6	14
152	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
151	Controlled tautomeric switching in azonaphthols tuned by substituents on the phenyl ring. *ChemPhysChem*, **2015**, 16, 649-57	3.2	13
150	Range-separated hybrid and double-hybrid density functionals: A quest for the determination of the range-separation parameter. *Journal of Chemical Physics*, **2020**, 152, 244124	3.9	13
149	Assessing modern GGA functionals for solids. *Journal of Molecular Modeling*, **2013**, 19, 2791-6	2	13
148	Ethylene dimerization catalyzed by mixed phosphine-iminophosphorane nickel(II) complexes: a DFT investigation. *Journal of Molecular Modeling*, **2013**, 19, 2107-18	2	13
147	A mechanistic and experimental study on the diethyl ether oxidation. *Process Safety Progress*, **2014**, 33, 64-69	1	13
146	Covalent vs electrostatic interactions in rare earth systems: a comparative study of U(III), U(IV), and U(V) and Nd(III) bonding properties by DFT and CAS-PT2 approaches. *Journal of Physical Chemistry A* , **2009**, 113, 14760-5	2.8	13
145	Bridging the gap between the topological and orbital description of hydrogen bonding: the case of the formic acid dimer and its sulfur derivatives. *Journal of Physical Chemistry A*, **2006**, 110, 5102-7	2.8	13
144	A theoretical study of the competition between ethylene insertion and chain transfer in cationic aluminum systems. *Chemical Physics Letters*, **2000**, 329, 99-105	2.5	13
143	The Oxidation of Thiols by Cobalt N4 Complexes: a Correlation between Theory and Experiments. *Journal of Physical Chemistry A*, **2001**, 105, 11304-11311	2.8	13
142	Modeling Polymerization Reactions at Aluminum-Based Catalysts: Is DFT a Reliable Computational Tool?. *Journal of Physical Chemistry A*, **2001**, 105, 9014-9023	2.8	13
141	Oximine form of the peptide bond as a transient modification in enzyme redox reactions. *The Journal of Physical Chemistry*, **1991**, 95, 4231-4238		13
140	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
139	Theoretical approaches for predicting the color of rigid dyes in solution. *Journal of Computational Chemistry*, **2017**, 38, 998-1004	3.5	12

138	Describing excited states of [n]cycloparaphenylenes by hybrid and double-hybrid density functionals: from isolated to weakly interacting molecules. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	12
137	Mixed lithium-sodium (LiNaCO3) and lithium-potassium (LiKCO3) carbonates for low temperature electrochemical applications: Structure, electronic properties and surface reconstruction from ab-initio calculations. *Surface Science*, **2016**, 647, 66-77	1.8	12
136	Structure of genipin in solution: a combined experimental and theoretical study. *RSC Advances*, **2013**, 3, 13764	3.7	12
135	Assessing the performances of some recently proposed density functionals for the description of organometallic structures. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	12
134	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
133	IR fingerprints of U(VI) nitrate monoamides complexes: a joint experimental and theoretical study. *Journal of Physical Chemistry A*, **2010**, 114, 10878-84	2.8	12
132	A theoretical investigation of the dye-redox mediator interaction in dye-sensitized photovoltaic cells. *Chemical Physics Letters*, **2003**, 371, 378-385	2.5	12
131	Environment effects on the oxidation of thiols: cobalt phthalocyanine as a test case. *Chemical Physics Letters*, **2003**, 376, 690-697	2.5	12
130	A theoretical investigation of gadolinium (III) solvation in molten salts. *Journal of Chemical Physics*, **2005**, 122, 224512	3.9	12
129	Semiconducting and optical properties of selected binary compounds by linear response DFT+U and hybrid functional methods. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	12
128	Aggregation Effects on Pigment Coatings: Pigment Red 179 as a Case Study. *ACS Omega*, **2019**, 4, 20315−20323	3.9	12
127	Theoretical and Experimental Study of the Reaction between Ammonium Nitrate and Sodium Salts. *Industrial & Engineering Chemistry Research*, **2016**, 55, 12183-12190	3.9	11
126	From iridoids to dyes: a theoretical study on genipin reactivity. *RSC Advances*, **2014**, 4, 11029	3.7	11
125	Oxidation mechanism of aliphatic ethers: theoretical insights on the main reaction channels. *Journal of Physical Chemistry A*, **2012**, 116, 9010-9	2.8	11
124	A DFT study of magnetic interactions in photoswitchable systems. *Chemical Physics Letters*, **2012**, 542, 13-18	2.5	11
123	Experimental evidence of correlation between 1/fnoise level and metal-to-insulator transition temperature in epitaxial La0.7Sr0.3MnO3thin films. *Journal Physics D: Applied Physics*, **2013**, 46, 202001	3	11
122	Toward an Accurate Modeling of the Water−Zeolite Interaction: Calibrating the DFT Approach. *Journal of Physical Chemistry Letters*, **2010**, 1, 763-768	6.4	11
121	Can molecular quantum descriptors predict the butene selectivity in nickel(II) catalyzed ethylene dimerization? A QSPR study. *International Journal of Quantum Chemistry*, **2010**, 110, 540-548	2.1	11

120	Assessing the performances of some recently proposed density functionals for the description of bond dissociations involving organic radicals. *International Journal of Quantum Chemistry*, **2010**, 110, 2320-2329	2.1	11
119	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
118	Capillary electrophoresis of inorganic anions in hydro-organic media. Influence of ion-pairing and solvation phenomena. *Journal of Chromatography A*, **2004**, 1032, 149-58	4.5	11
117	Solvent Effect on Density Functional Reactivity Indexes Applied to Substituted Nickel Phthalocyanines. *Journal of Physical Chemistry A*, **2004**, 108, 6045-6051	2.8	11
116	Description of the metal ligand bonding in f-element complexes: A DFT study including scalar relativistic effects. *International Journal of Quantum Chemistry*, **2003**, 91, 321-327	2.1	11
115	Stationary point structure and energetics: Density functional study including solvent effects on the tautomerization of formamide and 2-pyridone. *International Journal of Quantum Chemistry*, **1995**, 56, 645-653	2.1	11
114	A qualitative model to identify non-radiative decay channels: the spiropyran as case study. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	11
113	Optoeletronic properties of poly(N-alkenyl-carbazole)s driven by polymer stereoregularity. *Journal of Polymer Science Part A*, **2018**, 56, 242-251	2.5	11
112	The diene isomerization energies dataset: A difficult test for double-hybrid density functionals?. *Journal of Chemical Physics*, **2015**, 142, 224105	3.9	10
111	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
110	22 Electrons [1.1.1.1.1] pentaphyrin as a new photosensitizing agent for water disinfection: experimental and theoretical characterization. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	10
109	Molecular dynamics simulations of a lithium/sodium carbonate mixture. *Journal of Molecular Modeling*, **2016**, 22, 61	2	10
108	Modeling Chemical Incompatibility: Ammonium Nitrate and Sodium Salt of Dichloroisocyanuric Acid as a Case Study. *Industrial & Engineering Chemistry Research*, **2014**, 53, 13920-13927	3.9	10
107	Backbone effects on the charge transport in poly-imidazole membranes: a theoretical study. *Journal of Materials Chemistry A*, **2013**, 1, 7751	13	10
106	Modeling the Modulation of Emission Behavior in E/Z Isomers of Dipyrrolyldiphenylethene: From Molecules to Nanoaggregates. *Journal of Physical Chemistry C*, **2017**, 121, 25603-25616	3.8	10
105	Vibrational behavior of tetrahedral d0 oxo-compounds: A theoretical study. *Chemical Physics Letters*, **2006**, 429, 52-57	2.5	10
104	Solvent effects on molecular reactivity descriptors: some test cases. *Theoretical Chemistry Accounts* , **2004**, 111, 188-195	1.9	10
103	Structural and energetic characteristics of electron deficient M2H6 compounds from a density functional approach. *Chemical Physics Letters*, **1994**, 222, 597-602	2.5	10

102	Proton transfer in excited electronic states: environmental effects on the tautomerization of 2-pyridone. *Journal of Photochemistry and Photobiology A: Chemistry*, **1994**, 80, 211-219	4.7	10
101	Origin and fine tuning of the stability of five-coordinated platinum(II) and palladium(II) species. A quantum-mechanical study. *Inorganica Chimica Acta*, **1995**, 238, 159-163	2.7	10
100	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
99	Excited-State Proton Transfer and Intramolecular Charge Transfer in 1,3-Diketone Molecules. *ChemPhysChem*, **2016**, 17, 1530-8	3.2	10
98	In Silico Prediction of Catalytic Oligomerization Degrees. *Organometallics*, **2011**, 30, 3911-3914	3.8	9
97	Density-functional calculations for large systems: can GGA functionals be competitive with hybrid functionals?. *Interdisciplinary Sciences, Computational Life Sciences*, **2010**, 2, 163-8	3.5	9
96	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
95	A first combined electrochemical and modelling strategy on composite carbonate/oxide electrolytes for hybrid fuel cells. *International Journal of Hydrogen Energy*, **2016**, 41, 18778-18787	6.7	8
94	Representation of potential energy surfaces by discrete polynomials: proton transfer in malonaldehyde. *Physical Chemistry Chemical Physics*, **2000**, 2, 4095-4103	3.6	8
93	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
92	Hybrid Fuel Cells with Carbonate/Oxide Composite Electrolytes: An Electrochemical and Theoretical Insight. *ECS Transactions*, **2015**, 68, 2597-2609	1	7
91	Nonempirical (double-hybrid) density functionals applied to atomic excitation energies: A systematic basis set investigation. *International Journal of Quantum Chemistry*, **2020**, 120, e26193	2.1	7
90	Density Functional Determination of the Energetics of the Formation of trans-Stilbene Catalyzed by Sulfenate Anions. *ChemCatChem*, **2017**, 9, 278-281	5.2	7
89	Response to Comment on Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0 [J. Chem. Phys. 143, 187101 (2015)]. *Journal of Chemical Physics*, **2015**, 143, 187102	3.9	7
88	How the choice of a computational model could rule the chemical interpretation: the Ni(II) catalyzed ethylene dimerization as a case study. *Journal of Computational Chemistry*, **2010**, 31, 1053-62	3.5	7
87	Optimized GGA functional for proton transfer reactions. *Journal of Physical Chemistry A*, **2009**, 113, 14415-9	2.8	7
86	A comparative post-Hartree–Fock and density functional theory study of monochalcogenide diatomic molecules. *Computational and Theoretical Chemistry*, **2008**, 863, 79-83		7
85	Modelling the UV/visible spectrum of tetrakis(phenylethynyl)benzene. *Computational and Theoretical Chemistry*, **2008**, 863, 123-127		7

84	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
83	Static and dynamic descriptions of bond breaking/formation: a complementary view?. *Journal of Chemical Physics*, **2005**, 123, 211103	3.9	7
82	H2 Dissociation and Water Evolution on Silver-Decorated CeO2(111): A Hybrid Density Functional Theory Investigation. *Journal of Physical Chemistry C*, **2019**, 123, 25668-25679	3.8	6
81	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
80	Defect Formation and Diffusion on the (001) Surface of LiKCO3 for Fuel Cell Applications: Insight from Hybrid DFT. *Journal of Physical Chemistry C*, **2016**, 120, 12941-12951	3.8	6
79	Dithieno[3,2-b:2?,3?-d]pyran-containing organic D□A sensitizers for dye-sensitized solar cells. *RSC Advances*, **2014**, 4, 62472-62475	3.7	6
78	Toward tailorable surfaces: a combined theoretical and experimental study of lanthanum niobate layered perovskites. *Journal of Chemical Physics*, **2014**, 141, 024704	3.9	6
77	La0.7Sr0.3MnO3 thin films on SrTiO3 and CaTiO3 buffered Si substrates: structural, static, and dynamic magnetic properties. *Journal of Nanoparticle Research*, **2011**, 13, 5669-5675	2.3	6
76	General computational strategy to study polymerization reactions at aluminum-based catalysts. *International Journal of Quantum Chemistry*, **2003**, 91, 474-482	2.1	6
75	Proton transfer in the ground and excited electronic states of [2,2?-bipyridyl]-3,3?-diol. A semiempirical study. *Journal of the Chemical Society Perkin Transactions II*, **1995**, 1141-1147		6
74	Violation of Hund's rule in molecules: Predicting the excited-state energy inversion by TD-DFT with double-hybrid methods.. *Journal of Chemical Physics*, **2022**, 156, 034105	3.9	6
73	O2 Activation over Ag-Decorated CeO2(111) and TiO2(110) Surfaces: A Theoretical Comparative Investigation. *Journal of Physical Chemistry C*, **2020**, 124, 25917-25930	3.8	6
72	Modeling composite electrolytes for low-temperature solid oxide fuel cell application: structural, vibrational and electronic features of carbonate□oxide interfaces. *Journal of Materials Chemistry A*, **2016**, 4, 17473-17482	13	6
71	Understanding the properties of dithienylethenes functionalized for supramolecular self-assembly: a molecular modeling study. *Physical Chemistry Chemical Physics*, **2020**, 22, 6942-6952	3.6	5
70	Theoretical and Experimental Study on the Inhibition of Diethyl Ether Oxidation. *Energy & Fuels*, **2014**, 28, 2821-2829	4.1	5
69	New range-separated hybrids based on the TCA density functional. *Chemical Physics Letters*, **2012**, 519-520, 145-149	2.5	5
68	Effects of Anthryl Groups on the Charge Transport and Photovoltaic Properties of Small Triarylamine-Based Donor-Acceptor Molecules: A Joint Experimental and Theoretical Study. *ChemistrySelect*, **2017**, 2, 6296-6303	1.8	5
67	Atomic Structure and Properties of Charged Domain Walls in BiFeO3 Films. *Microscopy and Microanalysis*, **2013**, 19, 1654-1655	0.5	5

66	New Correlation Functionals In DFT: Theory And Tests **2009**,		5
65	Theoretical Study of Sticking Processes on Molecular Models of Silica Surfaces. *Theoretical Chemistry Accounts*, **2006**, 115, 379-384	1.9	5
64	Intrinsic Electric Transport in CMR Thin-Films. *Journal of Superconductivity and Novel Magnetism*, **2005**, 18, 719-722		5
63	Reply to the Comment "A theoretical study of bonding in lanthanide trihalides by density functional methods" by M. Hargittai. *Journal of Physical Chemistry A*, **1999**, 103, 7554-7554	2.8	5
62	Solvent effects on isomerization equilibria: An energetic analysis in the framework of density functional theory. *Theoretica Chimica Acta*, **1995**, 91, 199-214		5
61	Electrochemical synthesis of tetrakis[N-methylbenzothiazole-2(3H)-selone]selenium(2+) tetrafluroborate: an uncommon dication containing the mixed-valence Se5 framework. *Chemical Communications*, **1996**, 873	5.8	5
60	ESR features of the bicyclobutyl radical revisited. A counterintuitive ordering of short- and long-range isotropic hyperfine coupling constants. *Chemical Physics Letters*, **1995**, 246, 53-58	2.5	5
59	Development of Simple QSPR Models for the Prediction of the Heat of Decomposition of Organic Peroxides. *Molecular Informatics*, **2017**, 36, 1700024	3.8	4
58	In Silico Investigation of the Aggregation-Caused Quenching: the "Tolane-Based Molecule" Case. *ChemPhotoChem*, **2019**, 3, 794-803	3.3	4
57	Investigating the role of the "bridge characteristics in donor"spacer"acceptor type dyes for solar cell application: a theoretical study. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	4
56	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
55	In silico assessment of the HPLC"UV response coefficients. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 1-5	2	4
54	Subterahertz Momentum Drag and Violation of Matthiessen's Rule in an Ultraclean Ferromagnetic SrRuO_{3} Metallic Thin Film. *Physical Review Letters*, **2020**, 125, 217401	7.4	4
53	Investigation of ferromagnetic heterogeneities in La0.7Sr0.3MnO3thin films. *Journal Physics D: Applied Physics*, **2017**, 50, 045001	3	3
52	Gradient-regulated connection-based correction for the PBE exchange: the PBEtrans model. *Molecular Physics*, **2016**, 114, 1059-1065	1.7	3
51	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
50	Theoretical insights into inorganic-organic intercalation products of the layered perovskite HLaNbO: perspectives for hybrid proton conductors. *Physical Chemistry Chemical Physics*, **2019**, 21, 16647-16657	3.6	3
49	Simulations of UV"visible spectra for analytical applications: phenothiazines as a case study. *Molecular Simulation*, **2014**, 40, 169-175	2	3

48	Adsorption of successive layers of H2 molecules on a model copper surface: performances of second- to fifth-rung exchange-correlation functionals. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	3
47	Structural and Dynamical Features of Hydrogen Bonds from Conventional and Hybrid Density Functional Methods. *Recent Advances in Computational*, **1997**, 115-164		3
46	Beyond Chemical Accuracy for Alkane Thermochemistry: The DH Approach. *Journal of Organic Chemistry*, **2021**, 86, 5538-5545	4.2	3
45	Design, synthesis, biological evaluation, NMR and DFT studies of structurally simplified trimethoxy benzamides as selective P-glycoprotein inhibitors: the role of molecular flatness. *Chemical Biology and Drug Design*, **2016**, 88, 820-831	2.9	3
44	Electronic Energy and Local Property Errors at QTAIM Critical Points while Climbing Perdew's Ladder of Density-Functional Approximations.. *Journal of Chemical Theory and Computation*, **2021**,	6.4	3
43	Defect interaction and local structural distortions in Mg-doped LaGaO: A combined experimental and theoretical study. *Journal of Chemical Physics*, **2017**, 147, 144702	3.9	2
42	Interaction of osmium(ii) redox probes with DNA: insights from theory. *Physical Chemistry Chemical Physics*, **2016**, 18, 30029-30039	3.6	2
41	Communication: Accurate description of interaction energies and three-body effects in weakly bound molecular complexes by PBE-QIDH models. *Journal of Chemical Physics*, **2018**, 149, 041101	3.9	2
40	Theoretical study of direct and water-assisted isomerization of formaldehyde radical cation. A comparison between density functional and post-Hartree–Fock approaches (Chem. Phys. Letters 224 (1994) 432). *Chemical Physics Letters*, **1994**, 228, 499	2.5	2
39	Chemistry of ethanediyl S,S-acetals 6- An example of vicarious nucleophilic substitution of hydrogen in 1,4-benzodithians. *Tetrahedron*, **1993**, 49, 11383-11388	2.4	2
38	Stability of the polyynic form of C, C, C, and C nanorings: a challenge tackled by range-separated double-hybrid density functionals.. *Physical Chemistry Chemical Physics*, **2022**,	3.6	2
37	Intrinsic and Environmental Effects on Protomeric Equilibria in the Ground and Excited Electronic States of Biological Systems. *Topics in Molecular Organization and Engineering*, **1994**, 1-18		2
36	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
35	Electronic coupling in the reduced state lies at the origin of color changes of ommochromes. *Dyes and Pigments*, **2021**, 185, 108661	4.6	2
34	Mechanochromic LLDPE Films Doped with NIR Reflective Paliogen Black. *Macromolecular Rapid Communications*, **2021**, 42, e2000426	4.8	2
33	Determining the role of the underlying orbital-dependence of PBE0-DH and PBE-QIDH double-hybrid density functionals. *Journal of Computational Chemistry*, **2017**, 38, 1509-1514	3.5	1
32	Experimental and theoretical assignments of stereoregular poly(N-pentenylcarbazole) FT-IR spectra. *Vibrational Spectroscopy*, **2019**, 101, 64-70	2.1	1
31	Toward the Mechanistic Understanding of the Additives' Role on Ammonium Nitrate Decomposition: Calcium Carbonate and Calcium Sulfate as Case Studies. *ACS Omega*, **2020**, 5, 5034-5040	3.9	1

30	Dioxygenation of metal(II)-cysteinato complexes in CDO biomimetic models: Can ruthenium and osmium reach iron performances?. *International Journal of Quantum Chemistry*, **2018**, 118, e25525	2.1	1
29	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
28	Probing the performances of HISS functionals for the description of excited states of molecular systems. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	1
27	In-Situ Cross-Sectional Switching of Multiferroic BiFeO3 Thin Films. *Microscopy and Microanalysis*, **2011**, 17, 1360-1361	0.5	1
26	A theoretical investigation on the interaction of a new gene vector with DNA. *Theoretical Chemistry Accounts*, **2008**, 120, 507-513	1.9	1
25	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
24	Modeling Photonastic Materials: A First Computational Study. *Journal of Chemical Theory and Computation*, **2020**, 16, 7017-7032	6.4	1
23	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
22	Aggregation-Induced Emission: A Challenge for Computational Chemistry Taking TPA-BMO as an Example*. *ChemPhysChem*, **2021**, 22, 1802-1816	3.2	1
21	Pairing double hybrid functionals with a tailored basis set for an accurate thermochemistry of hydrocarbons.. *RSC Advances*, **2021**, 11, 26073-26082	3.7	1
20	A global analysis of excited states: the global transition contribution grids. *Theoretical Chemistry Accounts*, **2021**, 140, 1	1.9	0
19	Theoretical insights on acceptor-donor dyads for organic photovoltaics. *Physical Chemistry Chemical Physics*, **2020**, 22, 27413-27424	3.6	0
18	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
17	Tackling an accurate description of molecular reactivity with double-hybrid density functionals.. *Journal of Chemical Physics*, **2022**, 156, 161101	3.9	0
16	Mechanical and Electrical Control of Charged Domain Walls in Ferroelectric Materials. *Microscopy and Microanalysis*, **2014**, 20, 1546-1547	0.5	
15	Towards a Greater Accuracy in DFT Calculations: From GGA to Hybrid Functionals **2012**, 3-15		
14	Preface to the special collection in honour of Vincenzo Barone. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	
13	2-D Mapping of Ferroelectric Domains by Transmission Electron Microscopy. *Microscopy and Microanalysis*, **2011**, 17, 1356-1357	0.5	

12	Atomic Resolution Studies of Self-Stabilizing Metal-Perovskite Catalysts. *Microscopy and Microanalysis*, **2011**, 17, 1594-1595	0.5
11	The Contribution of Theoretical Chemistry to the Drug Design in Photodynamic Therapy **2011**, 121-134	
10	Interface Effects on Static and Dynamic Properties of Multiferroic BiFeO3. *Microscopy and Microanalysis*, **2012**, 18, 320-321	0.5
9	New Insight into Atomic Scale Phenomena in Novel Perovskite-Based Catalysts. *Microscopy and Microanalysis*, **2012**, 18, 1296-1297	0.5
8	ZnO Epitaxy on (111) Silicon Using Intervening Bixbyite Oxide Buffer Layers. *Microscopy and Microanalysis*, **2010**, 16, 1402-1403	0.5
7	On the nature of the cobalt-nitrogen bond in the CON+2 complex. A theoretical study. *Chemical Physics Letters*, **1996**, 254, 314-320	2.5
6	Adsorption of successive layers of H2 molecules on a model copper surface: performances of second- to fifth-rung exchange-correlation functionals. *Highlights in Theoretical Chemistry*, **2013**, 281-289	
5	Generalized gradient exchange functionals based on the gradient-regulated connection: a new member of the TCA family. *Highlights in Theoretical Chemistry*, **2013**, 237-243	
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	Role of Computational Variables on the Performances of COSMO-SAC Model: A Combined Theoretical and Experimental Investigation. *Industrial & Engineering Chemistry Research*, **2021**, 60, 2314-2325	3.9