Carlo Adamo

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	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
442	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
441	Tackling an accurate description of molecular reactivity with double-hybrid density functionals.. *Journal of Chemical Physics*, **2022**, 156, 161101	3.9	0
440	A global analysis of excited states: the global transition contribution grids. *Theoretical Chemistry Accounts*, **2021**, 140, 1	1.9	0
439	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
438	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
437	Beyond Chemical Accuracy for Alkane Thermochemistry: The DH Approach. *Journal of Organic Chemistry*, **2021**, 86, 5538-5545	4.2	3
436	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
435	Aggregation-Induced Emission: A Challenge for Computational Chemistry Taking TPA-BMO as an Example*. *ChemPhysChem*, **2021**, 22, 1802-1816	3.2	1
434	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	
433	Electronic coupling in the reduced state lies at the origin of color changes of ommochromes. *Dyes and Pigments*, **2021**, 185, 108661	4.6	2
432	Mechanochromic LLDPE Films Doped with NIR Reflective Paliogen Black. *Macromolecular Rapid Communications*, **2021**, 42, e2000426	4.8	2
431	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	
430	Pairing double hybrid functionals with a tailored basis set for an accurate thermochemistry of hydrocarbons.. *RSC Advances*, **2021**, 11, 26073-26082	3.7	1
429	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
428	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
427	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

426	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
425	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
424	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
423	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
422	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
421	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
420	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
419	Theoretical insights on acceptor-donor dyads for organic photovoltaics. *Physical Chemistry Chemical Physics*, **2020**, 22, 27413-27424	3.6	0
418	Modeling the Electron Transfer Chain in an Artificial Photosynthetic Machine. *Journal of Physical Chemistry Letters*, **2020**, 11, 9738-9744	6.4	
417	Modeling Photonastic Materials: A First Computational Study. *Journal of Chemical Theory and Computation*, **2020**, 16, 7017-7032	6.4	1
416	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
415	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
414	Range-separated hybrid density functionals made simple. *Journal of Chemical Physics*, **2019**, 150, 201102	3.9	40
413	In Silico Investigation of the Aggregation-Caused Quenching: the Tolane-Based Molecule Case. *ChemPhotoChem*, **2019**, 3, 794-803	3.3	4
412	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
411	Experimental and theoretical assignments of stereoregular poly(N-pentenylcarbazole) FT-IR spectra. *Vibrational Spectroscopy*, **2019**, 101, 64-70	2.1	1
410	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
409	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

408	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
407	sp-hybridized carbon allotrope molecular structures: An ongoing challenge for density-functional approximations. *Journal of Chemical Physics*, **2019**, 151, 211104	3.9	22
406	Aggregation Effects on Pigment Coatings: Pigment Red 179 as a Case Study. *ACS Omega*, **2019**, 4, 20315-20323	3.7	12
405	Does the gradient-regulated connection improve the description of correlated metal bond properties?. *International Journal of Quantum Chemistry*, **2019**, 119, e25831	2.1	
404	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
403	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
402	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
401	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
400	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
399	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
398	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
397	Accuracy of TD-DFT Geometries: A Fresh Look. *Journal of Chemical Theory and Computation*, **2018**, 14, 3715-3727	6.4	40
396	Range-Separated Double-Hybrid Functional from Nonempirical Constraints. *Journal of Chemical Theory and Computation*, **2018**, 14, 4052-4062	6.4	32
395	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
394	Investigation of ferromagnetic heterogeneities in La0.7Sr0.3MnO3thin films. *Journal Physics D: Applied Physics*, **2017**, 50, 045001	3	3
393	Theoretical approaches for predicting the color of rigid dyes in solution. *Journal of Computational Chemistry*, **2017**, 38, 998-1004	3.5	12
392	Understanding Aggregation-Induced Emission in Molecular Crystals: Insights from Theory. *Journal of Physical Chemistry C*, **2017**, 121, 5747-5752	3.8	37
391	Partnering dispersion corrections with modern parameter-free double-hybrid density functionals. *Physical Chemistry Chemical Physics*, **2017**, 19, 13481-13487	3.6	16

390	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
389	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
388	Development of Simple QSPR Models for the Prediction of the Heat of Decomposition of Organic Peroxides. *Molecular Informatics*, **2017**, 36, 1700024	3.8	4
387	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
386	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
385	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
384	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
383	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
382	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
381	Charge transfer excitations in TDDFT: A ghost-hunter index. *Journal of Computational Chemistry*, **2017**, 38, 2151-2156	3.5	30
380	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
379	Density Functional Determination of the Energetics of the Formation of trans-Stilbene Catalyzed by Sulfenate Anions. *ChemCatChem*, **2017**, 9, 278-281	5.2	7
378	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
377	Unveiling the Reactivity of a Synthetic Mimic of the Oxygen Evolving Complex. *Journal of Physical Chemistry Letters*, **2016**, 7, 5015-5021	6.4	15
376	Anchoring groups for dyes in p-DSSC application: insights from DFT. *Journal of Molecular Modeling*, **2016**, 22, 289	2	16
375	Interaction of osmium(ii) redox probes with DNA: insights from theory. *Physical Chemistry Chemical Physics*, **2016**, 18, 30029-30039	3.6	2
374	Theoretical and Experimental Study of the Reaction between Ammonium Nitrate and Sodium Salts. *Industrial & Engineering Chemistry Research*, **2016**, 55, 12183-12190	3.9	11
373	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

372	Quadratic integrand double-hybrid made spin-component-scaled. *Journal of Chemical Physics*, **2016**, 144, 124104	3.9	27
371	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
370	Gradient-regulated connection-based correction for the PBE exchange: the PBEtrans model. *Molecular Physics*, **2016**, 114, 1059-1065	1.7	3
369	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
368	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
367	Exploring the limits of recent exchange‐correlation functionals in modeling lithium/benzene interaction. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	20
366	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
365	Investigating the role of the π-bridge characteristics in donor–spacer–acceptor type dyes for solar cell application: a theoretical study. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	4
364	Modeling the photosensitizing properties of thiolate-protected gold nanoclusters. *Physical Chemistry Chemical Physics*, **2016**, 18, 7737-50	3.6	15
363	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
362	Molecular dynamics simulations of a lithium/sodium carbonate mixture. *Journal of Molecular Modeling*, **2016**, 22, 61	2	10
361	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
360	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
359	Computational Molecular Electronic Spectroscopy with TD-DFT. *Topics in Current Chemistry*, **2016**, 368, 347-75		25
358	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
357	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
356	Modeling emission features of salicylidene aniline molecular crystals: A QM/QM' approach. *Journal of Computational Chemistry*, **2016**, 37, 861-70	3.5	21
355	Excited-State Proton Transfer and Intramolecular Charge Transfer in 1,3-Diketone Molecules. *ChemPhysChem*, **2016**, 17, 1530-8	3.2	10

354	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
353	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
352	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
351	Modeling composite electrolytes for low-temperature solid oxide fuel cell application: structural, vibrational and electronic features of carbonate□xide interfaces. *Journal of Materials Chemistry A*, **2016**, 4, 17473-17482	13	6
350	Benchmarking the DFT methodology for assessing antioxidant-related properties: quercetin and edaravone as case studies. *Journal of Molecular Modeling*, **2016**, 22, 250	2	18
349	Nonempirical Double-Hybrid Functionals: An Effective Tool for Chemists. *Accounts of Chemical Research*, **2016**, 49, 1503-13	24.3	75
348	A qualitative model to identify non-radiative decay channels: the spiropyran as case study. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	11
347	Hybrid Fuel Cells with Carbonate/Oxide Composite Electrolytes: An Electrochemical and Theoretical Insight. *ECS Transactions*, **2015**, 68, 2597-2609	1	7
346	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
345	Exploring excited states using Time Dependent Density Functional Theory and density-based indexes. *Coordination Chemistry Reviews*, **2015**, 304-305, 166-178	23.2	94
344	Functionalized Graphene as an Electron-Cascade Acceptor for Air-Processed Organic Ternary Solar Cells. *Advanced Functional Materials*, **2015**, 25, 3870-3880	15.6	63
343	Theoretical Investigation of Hole Transporter Materials for Energy Devices. *Journal of Physical Chemistry C*, **2015**, 119, 23890-23898	3.8	37
342	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
341	The diene isomerization energies dataset: A difficult test for double-hybrid density functionals?. *Journal of Chemical Physics*, **2015**, 142, 224105	3.9	10
340	Systematic Improvement of Density Functionals through Parameter-Free Hybridization Schemes. *Journal of Physical Chemistry Letters*, **2015**, 6, 3540-5	6.4	34
339	A General Guidebook for the Theoretical Prediction of Physicochemical Properties of Chemicals for Regulatory Purposes. *Chemical Reviews*, **2015**, 115, 13093-164	68.1	87
338	Controlled tautomeric switching in azonaphthols tuned by substituents on the phenyl ring. *ChemPhysChem*, **2015**, 16, 649-57	3.2	13
337	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

336	Non-parametrized functionals with empirical dispersion corrections: A happy match?. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	16
335	A comprehensive DFT investigation of bulk and low-index surfaces of ZrO2 polymorphs. *Journal of Computational Chemistry*, **2015**, 36, 9-21	3.5	49
334	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
333	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
332	Computational Insights into Excited-State Proton-Transfer Reactions in Azo and Azomethine Dyes. *ChemPhysChem*, **2015**, 16, 3966-73	3.2	18
331	Intrinsic and dynamical reaction pathways of an excited state proton transfer. *Journal of Physical Chemistry B*, **2015**, 119, 2650-7	3.4	30
330	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
329	Effective electron displacements: a tool for time-dependent density functional theory computational spectroscopy. *Journal of Chemical Physics*, **2014**, 140, 104101	3.9	50
328	Theoretical and Experimental Study on the Inhibition of Diethyl Ether Oxidation. *Energy & Fuels*, **2014**, 28, 2821-2829	4.1	5
327	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
326	Dye chemistry with time-dependent density functional theory. *Physical Chemistry Chemical Physics*, **2014**, 16, 14334-56	3.6	225
325	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
324	Electronic Band Shapes Calculated with Optimally Tuned Range-Separated Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 4599-608	6.4	36
323	Dithieno[3,2-b:2?,3?-d]pyran-containing organic DA sensitizers for dye-sensitized solar cells. *RSC Advances*, **2014**, 4, 62472-62475	3.7	6
322	Intermolecular proton shuttling in excited state proton transfer reactions: insights from theory. *Physical Chemistry Chemical Physics*, **2014**, 16, 8661-6	3.6	33
321	Non-radiative decay paths in rhodamines: new theoretical insights. *Physical Chemistry Chemical Physics*, **2014**, 16, 20681-8	3.6	35
320	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
319	Oxidation of Ethylbenzene to Acetophenone with N-Doped Graphene: Insight from Theory. *Journal of Physical Chemistry C*, **2014**, 118, 12275-12284	3.8	31

318	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
317	From iridoids to dyes: a theoretical study on genipin reactivity. *RSC Advances*, **2014**, 4, 11029	3.7	11
316	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
315	Localized excited charge carriers generate ultrafast inhomogeneous strain in the multiferroic BiFeO3. *Physical Review Letters*, **2014**, 112, 097602	7.4	80
314	In silico assessment of the HPLC□UV response coefficients. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 1-5	2	4
313	Copper-amyloid-□complex may catalyze peroxynitrite production in brain: evidence from molecular modeling. *Physical Chemistry Chemical Physics*, **2014**, 16, 10169-74	3.6	14
312	Mechanical and Electrical Control of Charged Domain Walls in Ferroelectric Materials. *Microscopy and Microanalysis*, **2014**, 20, 1546-1547	0.5	
311	Simulations of UV□isible spectra for analytical applications: phenothiazines as a case study. *Molecular Simulation*, **2014**, 40, 169-175	2	3
310	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
309	Communication: double-hybrid functionals from adiabatic-connection: the QIDH model. *Journal of Chemical Physics*, **2014**, 141, 031101	3.9	108
308	Toward tailorable surfaces: a combined theoretical and experimental study of lanthanum niobate layered perovskites. *Journal of Chemical Physics*, **2014**, 141, 024704	3.9	6
307	A mechanistic and experimental study on the diethyl ether oxidation. *Process Safety Progress*, **2014**, 33, 64-69	1	13
306	Prediction of the thermal decomposition of organic peroxides by validated QSPR models. *Journal of Hazardous Materials*, **2014**, 276, 216-24	12.8	26
305	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
304	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
303	Backbone effects on the charge transport in poly-imidazole membranes: a theoretical study. *Journal of Materials Chemistry A*, **2013**, 1, 7751	13	10
302	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
301	Structure of genipin in solution: a combined experimental and theoretical study. *RSC Advances*, **2013**, 3, 13764	3.7	12

300	Assessing modern GGA functionals for solids. *Journal of Molecular Modeling*, **2013**, 19, 2791-6	2	13
299	Ethylene dimerization catalyzed by mixed phosphine-iminophosphorane nickel(II) complexes: a DFT investigation. *Journal of Molecular Modeling*, **2013**, 19, 2107-18	2	13
298	Evaluating push-pull dye efficiency using TD-DFT and charge transfer indices. *Physical Chemistry Chemical Physics*, **2013**, 15, 20210-9	3.6	53
297	Assessing the performances of some recently proposed density functionals for the description of organometallic structures. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	12
296	Discriminating role of bases in diketonate copper(I)-catalyzed C-O couplings: phenol versus diarylether. *Dalton Transactions*, **2013**, 42, 5348-54	4.3	32
295	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
294	Surface-dependent oxidation of H 2 on CeO 2 surfaces. *Journal of Catalysis*, **2013**, 297, 193-201	7.3	93
293	Communication: one third: a new recipe for the PBE0 paradigm. *Journal of Chemical Physics*, **2013**, 138, 021104	3.9	84
292	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
291	Modeling Dye-Sensitized Solar Cells: From Theory to Experiment. *Journal of Physical Chemistry Letters*, **2013**, 4, 1044-50	6.4	93
290	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
289	Photophysical properties of NIR-emitting fluorescence probes: insights from TD-DFT. *Physical Chemistry Chemical Physics*, **2013**, 15, 10019-27	3.6	29
288	The calculations of excited-state properties with Time-Dependent Density Functional Theory. *Chemical Society Reviews*, **2013**, 42, 845-56	58.5	1048
287	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
286	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
285	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
284	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
283	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

282	Exploring the metric of excited state proton transfer reactions. *Journal of Physical Chemistry B*, **2013**, 117, 16165-73	3.4	50
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