Juan C Sancho GarcÃ-a

List of Publications by Year
in descending order

149 papers	5,035 citations	81743 39 h-index	114278 63 g-index
152 all docs	152 docs citations	152 times ranked	4619 citing authors

#	Article	IF	Citations
1	Stabilizing and Modulating Color by Copigmentation: Insights from Theory and Experiment. Chemical Reviews, 2016, 116, 4937-4982.	23.0	408
2	Highly emissive excitons with reduced exchange energy in thermally activated delayed fluorescent molecules. Nature Communications, 2019, 10, 597.	5.8	253
3	Benchmarking Density Functionals on Structural Parameters of Small-/Medium-Sized Organic Molecules. Journal of Chemical Theory and Computation, 2016, 12, 459-465.	2.3	165
4	Electronic and optical properties of polyfluorene and fluorene-based copolymers: A quantum-chemical characterization. Journal of Chemical Physics, 2003, 118, 6615-6623.	1.2	160
5	Communication: Double-hybrid functionals from adiabatic-connection: The QIDH model. Journal of Chemical Physics, 2014, 141, 031101.	1.2	154
6	Computational Design of Thermally Activated Delayed Fluorescence Materials: The Challenges Ahead. Journal of Physical Chemistry Letters, 2018, 9, 6149-6163.	2.1	121
7	Theoretical Rationalization of the Singletâ€“Triplet Gap in OLEDs Materials: Impact of Charge-Transfer Character. Journal of Chemical Theory and Computation, 2015, 11, 168-177.	2.3	108
8	Large magnetic exchange coupling in rhombus-shaped nanographenes with zigzag periphery. Nature Chemistry, 2021, 13, 581-586.	6.6	104
9	Nonempirical Double-Hybrid Functionals: An Effective Tool for Chemists. Accounts of Chemical Research, 2016, 49, 1503-1513.	7.6	103
10	Nature of the singlet and triplet excitations mediating thermally activated delayed fluorescence. Physical Review Materials, 2017, 1, .	0.9	102
11	Double-hybrid density functionals: merging wavefunction and density approaches to get the best of both worlds. Physical Chemistry Chemical Physics, 2013, 15, 14581.	1.3	100
12	Dynamic nature of excited states of donorâ€“acceptor TADF materials for OLEDs: how theory can reveal structureâ€“property relationships. Journal of Materials Chemistry C, 2017, 5, 5718-5729.	2.7	97
13	Multireference coupled-cluster calculations on the energy of activation in the automerization of cyclobutadiene: Assessment of the state-specific multireference Brillouinâ€“Wigner theory. Journal of Chemical Physics, 2000, 112, 8785-8788.	1.2	93
14	Assessment of the reliability of the Perdewâ€“Burkeâ€“Ernzerhof functionals in the determination of torsional potentials in Ï€-conjugated molecules. Chemical Physics Letters, 2003, 377, 63-68.	1.2	74
15	Assessment of double-hybrid energy functionals for Ï€-conjugated systems. Journal of Chemical Physics, 2009, 131, 084108.	1.2	74
16	Highlights on Anthocyanin Pigmentation and Copigmentation: A Matter of Flavonoid Ï€-Stacking Complexation To Be Described by DFT-D. Journal of Chemical Theory and Computation, 2012, 8, 2034-2043.	2.3	71
17	Deep-Blue Oxadiazole-Containing Thermally Activated Delayed Fluorescence Emitters for Organic Light-Emitting Diodes. ACS Applied Materials & Interfaces, 2018, 10, 33360-33372.	4.0	67
18	Exchange Rules for Diradical Ï€-Conjugated Hydrocarbons. Nano Letters, 2019, 19, 5991-5997.	4.5	65

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19	Assessment of recently developed exchange-correlation functionals for the description of torsion potentials in Ï€-conjugated molecules. Journal of Chemical Physics, 2004, 121, 3096-3101.	1.2	63
20	Assessment of density-functional models for organic molecular semiconductors: The role of Hartreeâ€“Fock exchange in charge-transfer processes. Chemical Physics, 2007, 331, 321-331.	0.9	63
21	Three-Dimensional Energy Transport in Highly Luminescent Hostâ^'Guest Crystals:Â A Quantitative Experimental and Theoretical Study. Journal of the American Chemical Society, 2007, 129, 8585-8593.	6.6	62
22	Range-separated hybrid density functionals made simple. Journal of Chemical Physics, 2019, 150, 201102.	1.2	60
23	Modeling the Dynamics of Chromophores in Conjugated Polymers: The Case of Poly(2-methoxy-5-(2â€²-ethylhexyl)oxy 1,4-phenylene vinylene) (MEH-PPV). Journal of Physical Chemistry B, 2009, 113, 1311-1322.	1.2	59
24	Molecular packing and charge transport parameters in crystalline organic semiconductors from first-principles calculations. Physical Chemistry Chemical Physics, 2010, 12, 9381.	1.3	57
25	Improved accuracy with medium cost computational methods for the evaluation of bond length alternation of increasingly long oligoacetylenes. Physical Chemistry Chemical Physics, 2007, 9, 5874.	1.3	55
26	Nonlocal van der Waals Approach Merged with Double-Hybrid Density Functionals: Toward the Accurate Treatment of Noncovalent Interactions. Journal of Chemical Theory and Computation, 2013, 9, 3437-3443.	2.3	53
27	Effect of an external electric field on the charge transport parameters in organic molecular semiconductors. Journal of Chemical Physics, 2003, 119, 12563-12568.	1.2	49
28	Anchoring the Torsional Potential of Biphenyl at the ab Initio Level:â€‰ The Role of Basis Set versus Correlation Effects. Journal of Chemical Theory and Computation, 2005, 1, 581-589.	2.3	48
29	Accurate Treatment of Large Supramolecular Complexes by Double-Hybrid Density Functionals Coupled with Nonlocal van der Waals Corrections. Journal of Chemical Theory and Computation, 2015, 11, 932-939.	2.3	48
30	Charge-transport properties of prototype molecular materials for organic electronics based on graphene nanoribbons. Physical Chemistry Chemical Physics, 2009, 11, 2741.	1.3	47
31	Ab Initio Modeling of Donorâ€“Acceptor Interactions and Charge-Transfer Excitations in Molecular Complexes: The Case of Terthiopheneâ€“Tetracyanoquinodimethane. Journal of Chemical Theory and Computation, 2011, 7, 2068-2077.	2.3	46
32	Range-Separated Double-Hybrid Functional from Nonempirical Constraints. Journal of Chemical Theory and Computation, 2018, 14, 4052-4062.	2.3	45
33	Singletâ€Triplet Excitedâ€State Inversion in Heptazine and Related Molecules: Assessment of TDâ€DFT and ab initio Methods. ChemPhysChem, 2021, 22, 553-560.	1.0	45
34	Systematic Improvement of Density Functionals through Parameter-Free Hybridization Schemes. Journal of Physical Chemistry Letters, 2015, 6, 3540-3545.	2.1	44
35	A theoretical study of the molecular structure and torsional potential of styrene. Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, 1509-1523.	0.6	43
36	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.	1.2	41

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37	Negative Singletâ€“Triplet Excitation Energy Gap in Triangle-Shaped Molecular Emitters for Efficient Triplet Harvesting. Journal of Physical Chemistry A, 2021, 125, 513-522.	1.1	41
38	Design of Ï€-Conjugated Organic Materials for One-Dimensional Energy Transport in Nanochannels. Journal of Physical Chemistry B, 2005, 109, 4872-4880.	1.2	40
39	Accurate calculation of transport properties for organic molecular semiconductors with spin-component scaled MP2 and modern density functional theory methods. Journal of Chemical Physics, 2008, 129, 024103.	1.2	39
40	The role of topology in organic molecules: origin and comparison of the radical character in linear and cyclic oligoacenes and related oligomers. Physical Chemistry Chemical Physics, 2018, 20, 7112-7124.	1.3	39
41	Joint Theoretical and Experimental Characterization of the Structural and Electronic Properties of Poly(dioctylfluorene-alt-N-butylphenyl diphenylamine). Journal of Physical Chemistry B, 2004, 108, 5594-5599.	1.2	38
42	Torsional potential of 4,4â€²-bipyridine: Ab initio analysis of dispersion and vibrational effects. Journal of Chemical Physics, 2005, 123, 134309.	1.2	37
43	Is There Still Room for Parameter Free Double Hybrids? Performances of PBE0-DH and B2PLYP over Extended Benchmark Sets. Journal of Chemical Theory and Computation, 2013, 9, 3444-3452.	2.3	37
44	Synthesis of Axially Substituted Tetrapyrazinoporphyrazinato Metal Complexes for Optical Limiting and Study of Their Photophysical Properties. Journal of Physical Chemistry B, 2005, 109, 5425-5432.	1.2	35
45	Description of C(sp2)â^'C(sp2) Rotation in Butadiene by Density Functionals. Journal of Physical Chemistry A, 2001, 105, 11541-11548.	1.1	34
46	Assessing a new nonempirical density functional: Difficulties in treating Ï€-conjugation effects. Journal of Chemical Physics, 2006, 124, 124112.	1.2	34
47	Speed-Up of the Excited-State Benchmarking: Double-Hybrid Density Functionals as Test Cases. Journal of Chemical Theory and Computation, 2017, 13, 5539-5551.	2.3	33
48	Modeling of Multiresonant Thermally Activated Delayed Fluorescence Emittersâ”€Properly Accounting for Electron Correlation Is Key!. Journal of Chemical Theory and Computation, 2022, 18, 4903-4918.	2.3	32
49	A comparison between DFT and other ab initio schemes on the activation energy in the automerization of cyclobutadiene. Chemical Physics Letters, 2000, 317, 245-251.	1.2	31
50	Quadratic integrand double-hybrid made spin-component-scaled. Journal of Chemical Physics, 2016, 144, 124104.	1.2	31
51	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, 1756-1762.	1.1	31
52	Partnering dispersion corrections with modern parameter-free double-hybrid density functionals. Physical Chemistry Chemical Physics, 2017, 19, 13481-13487.	1.3	31
53	A theoretical study of Ï€-stacking tetracene derivatives as promising organic molecular semiconductors. Chemical Physics Letters, 2010, 499, 146-151.	1.2	29
54	sp-hybridized carbon allotrope molecular structures: An ongoing challenge for density-functional approximations. Journal of Chemical Physics, 2019, 151, 211104.	1.2	29

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55	Optical properties of wine pigments: theoretical guidelines with new methodological perspectives. Tetrahedron, 2015, 71, 3079-3088.	1.0	28
56	Synthesis, DFT calculations, linear and nonlinear optical properties of binuclear phthalocyanine gallium chloride. Journal of Molecular Modeling, 2006, 12, 543-550.	0.8	27
57	Nitrobenzene rotational energy barrier: A survey of several ab initio methods. Journal of Chemical Physics, 2003, 119, 5121-5127.	1.2	26
58	Assessment of Recently Developed Multicoefficient Strategies for the Treatment of Ï€-Conjugated Molecules. Journal of Physical Chemistry A, 2005, 109, 3470-3475.	1.1	26
59	Theoretical study of stability and charge-transport properties of coronene molecule and some of its halogenated derivatives: A path to ambipolar organic-based materials?. Journal of Chemical Physics, 2014, 141, 134708.	1.2	26
60	DLPNO-CCSD(T) scaled methods for the accurate treatment of large supramolecular complexes. Journal of Computational Chemistry, 2017, 38, 1869-1878.	1.5	26
61	Violation of Hundâ€™s rule in molecules: Predicting the excited-state energy inversion by TD-DFT with double-hybrid methods. Journal of Chemical Physics, 2022, 156, 034105.	1.2	26
62	Conductance Enhancement in Nanographeneâ^'Gold Junctions by Molecular Ï€-Stacking. Journal of the American Chemical Society, 2009, 131, 14857-14867.	6.6	25
63	Nearâ€Infrared Lasing in Fourâ€Zigzag Edged Nanographenes by 1D versus 2D Electronic Ï€â€Conjugation. Advanced Functional Materials, 2021, 31, 2105073.	7.8	25
64	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.	1.2	24
65	Formation of Cyclophane Macrocycles in Carbazole-Based Biradicaloids: Impact of the Dicyanomethylene Substitution Position. ACS Omega, 2019, 4, 4761-4769.	1.6	23
66	Precision Nanotube Mimics via Self-Assembly of Programmed Carbon Nanohoops. Journal of Organic Chemistry, 2020, 85, 129-141.	1.7	23
67	Theoretical Characterization and Design of End-Substituted Distyrylbenzenes as Excitation Shuttles in One-Dimensional Channels. Advanced Materials, 2004, 16, 1193-1197.	11.1	22
68	Dependence of Charge-Transport Parameters on Static Correlation and Self-Interaction Energy: The Case of a 1,4-Bis(Phenylethynyl)Benzene Derivative Conjugated Molecule. Journal of Physical Chemistry A, 2008, 112, 10325-10332.	1.1	22
69	Double Hybrid Functionals and the Î-System Bond Length Alternation Challenge: Rivaling Accuracy of Post-HF Methods. Journal of Chemical Theory and Computation, 2015, 11, 832-838.	2.3	22
70	Optoelectronic and Semiconducting Properties of Conjugated Polymers Composed of Thiazolo[5,4-d]thiazole and Arene Imides Linked by Ethynylene Bridges. Journal of Physical Chemistry C, 2016, 120, 24583-24596.	1.5	22
71	Assessing challenging intraâ€•and <scp>interâ€molecular chargeâ€transfer</scp> excitations energies with <scp>doubleâ€hybrid</scp> density functionals. Journal of Computational Chemistry, 2021, 42, 970-981.	1.5	22
72	Usefulness of the Colleâ€“Salvetti model for the treatment of the nondynamic correlation. Journal of Chemical Physics, 2003, 118, 1054-1058.	1.2	21

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73	Effect of Cyclic Topology on Charge-Transfer Properties of Organic Molecular Semiconductors: The Case of Cycloparaphenylene Molecules. Journal of Physical Chemistry C, 2016, 120, 9104-9111.	1.5	21
74	High-level ab initio calculations of the torsional potential of glyoxal. Chemical Physics Letters, 2001, 342, 452-460.	1.2	20
75	From cyclic nanorings to single-walled carbon nanotubes: disclosing the evolution of their electronic structure with the help of theoretical methods. Physical Chemistry Chemical Physics, 2019, 21, 2547-2557.	1.3	20
76	Torsional potential of 1,3-butadiene:ab initiocalculations. Molecular Physics, 2001, 99, 47-51.	0.8	19
77	Diastereoselective Synthesis of C₆₀/Steroid Conjugates. Journal of Organic Chemistry, 2013, 78, 2819-2826.	1.7	19
78	Bis(arylene-ethynylene)-s-tetrazines: A Promising Family of n-Type Organic Semiconductors?. Journal of Physical Chemistry C, 2015, 119, 18945-18955.	1.5	18
79	Computational Studies of Molecular Materials for Unconventional Energy Conversion: The Challenge of Light Emission by Thermally Activated Delayed Fluorescence. Molecules, 2020, 25, 1006.	1.7	18
80	New approach to the design of density functionals. Journal of Chemical Physics, 2001, 114, 2022-2026.	1.2	17
81	Obtaining the lattice energy of the anthracene crystal by modern yet affordable first-principles methods. Journal of Chemical Physics, 2013, 138, 204304.	1.2	17
82	The Nonlocal Correlation Density Functional VV10. Annual Reports in Computational Chemistry, 2015, 11, 37-102.	0.9	17
83	Cost-Effective Force Field Tailored for Solid-Phase Simulations of OLED Materials. Journal of Chemical Theory and Computation, 2015, 11, 3383-3392.	2.3	17
84	Theoretical Determination of Interaction and Cohesive Energies of Weakly Bound Cycloparaphenylene Molecules. Journal of Physical Chemistry C, 2016, 120, 22627-22634.	1.5	17
85	Non-parametrized functionals with empirical dispersion corrections: A happy match?. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	16
86	Charge transport parameters for carbon based nanohoops and donorâ€“acceptor derivatives. Physical Chemistry Chemical Physics, 2019, 21, 2057-2068.	1.3	16
87	The torsional potential in 2,2â€²-bipyrrole revisited: High-level ab initio and DFT results. Chemical Physics Letters, 2005, 411, 321-326.	1.2	15
88	Combining two-body density correlation functionals with multiconfigurational wave functions using natural orbitals and occupation numbers. Journal of Chemical Physics, 2007, 127, 104102.	1.2	15
89	Regio- and Stereocontrolled Synthesis of Oligostilbenoids: Theoretical Highlights at the Supramolecular Level. Journal of Natural Products, 2013, 76, 538-546.	1.5	15
90	Intraâ€•and Intermolecular Dispersion Interactions in [n]Cycloparaphenylenes: Do They Influence Their Structural and Electronic Properties?. ChemPhysChem, 2015, 16, 1520-1528.	1.0	15

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91	Electronic Energy and Local Property Errors at QTAIM Critical Points while Climbing Perdewâ€™s Ladder of Density-Functional Approximations. Journal of Chemical Theory and Computation, 2022, 18, 293-308.	2.3	14
92	Treatment of singletâ€“triplet splitting of a set of phenylene ethylenes organic molecules by TD-DFT. Chemical Physics Letters, 2007, 439, 236-242.	1.2	13
93	The diene isomerization energies dataset: A difficult test for double-hybrid density functionals?. Journal of Chemical Physics, 2015, 142, 224105.	1.2	13
94	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.	0.5	13
95	Understanding and Controlling Chemical Modifications of Rubicene for Their Envisioned Use as Molecular Organic Semiconductors. Journal of Physical Chemistry C, 2017, 121, 3171-3181.	1.5	13
96	Virtual Design in Organic Electronics: Screening of a Large Set of 1,4-Bis(phenylethynyl)benzene Derivatives as Molecular Semiconductors. Journal of Physical Chemistry C, 2017, 121, 28249-28261.	1.5	13
97	On the application of the Kohnâ€“Sham theory to the calculation of potential energy curves. Chemical Physics Letters, 1998, 288, 418-422.	1.2	12
98	Reliable DFT-based estimates of cohesive energies of organic solids: The anthracene crystal. Journal of Chemical Physics, 2012, 137, 194311.	1.2	12
99	Stability of the polyynic form of C₁₈, C₂₂, C₂₆, and C₃₀nanorings: a challenge tackled by range-separated double-hybrid density functionals. Physical Chemistry Chemical Physics, 2022, 24, 4515-4525.	1.3	12
100	Conformational Analysis of 2,2â€²-bifuran: Correlated High-level Ab initio and DFT Results. Theoretical Chemistry Accounts, 2006, 115, 427-433.	0.5	11
101	Ï€-Stacked polyphenolic dimers: A case study using dispersion-corrected methods. Chemical Physics Letters, 2013, 578, 120-125.	1.2	11
102	Double-Hybrid Functionals and Tailored Basis Set: Fullerene (C₆₀) Dimer and Isomers as Test Cases. Journal of Physical Chemistry A, 2019, 123, 10040-10046.	1.1	11
103	Dynamic Covalent Properties of a Novel Indolo[3,2â€•b]carbazole Diradical. Chemistry - A European Journal, 2021, 27, 5509-5520.	1.7	11
104	Application of double-hybrid density functionals to charge transfer in N-substituted pentacenequinones. Journal of Chemical Physics, 2012, 136, 174703.	1.2	10
105	Extending the applicability of the PBE0-DH double-hybrid model to weak interactions. Chemical Physics Letters, 2012, 535, 136-139.	1.2	10
106	Determining the cohesive energy of coronene by dispersion-corrected DFT methods: Periodic boundary conditions vs. molecular pairs. Journal of Chemical Physics, 2015, 142, 054702.	1.2	10
107	Nonempirical (doubleâ€hybrid) density functionals applied to atomic excitation energies: A systematic basis set investigation. International Journal of Quantum Chemistry, 2020, 120, e26193.	1.0	10
108	Beyond Chemical Accuracy for Alkane Thermochemistry: The DHthermo Approach. Journal of Organic Chemistry, 2021, 86, 5538-5545.	1.7	10

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109	A systematic and accurate study of singlet propynylidene1Part of this work was done at the J. HeyrovskÃ½ Institute of Physical Chemistry, Prague, Czech Republic.1. Chemical Physics Letters, 2000, 318, 649-654.	1.2	9
110	Using circumacenes to improve organic electronics and molecular electronics: design clues. Nanotechnology, 2009, 20, 475201.	1.3	9
111	A comparative study of modern and robust computational methods applied to <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si20.gif" display="inline" overflow="scroll"><mml:mrow><mml:mi mathvariant="normal">Ï€</mml:mi></mml:mrow></mml:math>-complexes of moderate size: The case of the ethene/benzenium ion complex. Chemical Physics Letters, 2009, 468, 138-142.	1.2	9
112	Theoretical approach to the conformational analysis of heteroaromatic dimers: 2-(2-Thienyl)pyrrole, 2-(2-thienyl)furan, and 2-(2-furyl)pyrrole. Chemical Physics Letters, 2009, 473, 49-56.	1.2	9
113	Oligostilbenoids from the Heartwood of N.â€¦Heimii: Role of Nonâ€Covalent Association in their Biogenesis. Chemistry - an Asian Journal, 2015, 10, 198-211.	1.7	9
114	Nâ€doped cycloparaphenylenes: Tuning electronic properties for applications in thermally activated delayed fluorescence. International Journal of Quantum Chemistry, 2018, 118, e25562.	1.0	9
115	Quantum-Chemical Insights into the Self-Assembly of Carbon-Based Supramolecular Complexes. Molecules, 2018, 23, 118.	1.7	9
116	Double Hybrids and Noncovalent Interactions: How Far Can We Go?. Journal of Physical Chemistry A, 2022, 126, 2590-2599.	1.1	9
117	Theoretical study of challenging properties of intramolecularly Ï€-stacked oligo(dibenzofulvene) organic molecular semiconductors. Theoretical Chemistry Accounts, 2010, 127, 605-612.	0.5	7
118	Studying physisorption processes and molecular friction of cycloparaphenylene molecules on graphene nano-sized flakes: role of Ï€â‹¯Ï€ and CHâ‹¯Ï€ interactions. Molecular Systems Design and Engineering, 2017, 2, 253-262.	1.7	7
119	Structure and Charge Transport Properties of Cycloparaphenylene Monolayers on Graphite. Advanced Materials Interfaces, 2019, 6, 1801948.	1.9	7
120	Combined Theoretical and Experimental Study on Intramolecular Charge Transfer Processes in Star-Shaped Conjugated Molecules. Journal of Physical Chemistry C, 2019, 123, 11179-11188.	1.5	7
121	Investigating the (Poly)Radicaloid Nature of Real-World Organic Compounds with DFT-Based Methods. Journal of Physical Chemistry A, 2020, 124, 3590-3600.	1.1	7
122	Computation of covalent and noncovalent structural parameters at low computational cost: Efficiency of the <scp>DHâ€SVPD</scp> method. International Journal of Quantum Chemistry, 2020, 120, e26233.	1.0	7
123	Tackling an accurate description of molecular reactivity with double-hybrid density functionals. Journal of Chemical Physics, 2022, 156, 161101.	1.2	7
124	Further evidences of the quality of double-hybrid energy functionals for Ï€-conjugated systems. Journal of Chemical Physics, 2011, 134, 234102.	1.2	6
125	Correlation factor approach to the correlation energy functional. Theoretical Chemistry Accounts, 2004, 111, 1-17.	0.5	5
126	On the role of the nonlocal Hartreeâ€“Fock exchange in ab initio quantum transport: H2 in Pt nanocontacts revisited. Journal of Chemical Physics, 2008, 129, 034702.	1.2	5

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127	Emerging DFT Methods and Their Importance for Challenging Molecular Systems with Orbital Degeneracy. Computation, 2019, 7, 62.	1.0	5
128	peri-Acenoacene molecules: tuning of the singlet and triplet excitation energies by modifying their radical character. Physical Chemistry Chemical Physics, 2021, 23, 24016-24028.	1.3	5
129	Organic Emitters Showing Excited-States Energy Inversion: An Assessment of MC-PDFT and Correlation Energy Functionals Beyond TD-DFT. Computation, 2022, 10, 13.	1.0	5
130	New correlation energy functionals with explicit dependence on the number of electrons. Journal of Chemical Physics, 2002, 116, 10571-10576.	1.2	4
131	Performance of multi-configurational calculations for a 1,4-bis(phenylethynyl)benzene derivative conjugated molecule. Physical Chemistry Chemical Physics, 2008, 10, 2308.	1.3	4
132	Extracting dimer structures from simulations of organic-based materials using QM/MM methods. Chemical Physics, 2015, 459, 112-124.	0.9	4
133	Theoretical Study of Cyclic Pyrene Oligomers and Their Resemblance with Cyclic Paraphenylenes: Disclosing Structureâ€“Property Relationships for Cyclic Nanorings. Journal of Physical Chemistry C, 2016, 120, 22069-22078.	1.5	4
134	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.	1.2	4
135	Theoretical Insights for Materials Properties of Cyclic Organic Nanorings. Advanced Theory and Simulations, 2020, 3, 2000110.	1.3	4
136	Pairing double hybrid functionals with a tailored basis set for an accurate thermochemistry of hydrocarbons. RSC Advances, 2021, 11, 26073-26082.	1.7	4
137	Tuning the Diradical Character of Indolocarbazoles: Impact of Structural Isomerism and Substitution Position. Journal of Physical Chemistry Letters, 2022, 13, 6003-6010.	2.1	4
138	Stability of Hydrocarbons of the Polyhedrane Family: Convergence of ab Initio Calculations and Corresponding Assessment of DFT Main Approximations. Journal of Chemical Theory and Computation, 2011, 7, 2761-2765.	2.3	3
139	A theoretical study of a strongly correlated linear H50 chain. Chemical Physics Letters, 2011, 511, 172-175.	1.2	3
140	Frustrated magnetic interactions in a cyclacene crystal. Physical Review Materials, 2022, 6, .	0.9	3
141	Unraveling the performance of dispersion-corrected functionals for the accurate description of weakly bound natural polyphenols. Journal of Molecular Modeling, 2015, 21, 291.	0.8	2
142	Determining the role of the underlying orbitalâ€dependence of PBE0â€DH and PBEâ€QIDH doubleâ€hybrid density functionals. Journal of Computational Chemistry, 2017, 38, 1509-1514.	1.5	2
143	The application of TD-DFT to excited states of a family of TPD molecules interesting for optoelectronic use. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	2
144	Reactivity of cycloparaphenylenes: Studying the possible growth of single-walled carbon nanotubes with DFT methods. Chemical Physics Letters, 2018, 697, 17-22.	1.2	2

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145	Nature (Hole or Electron) of Charge-Transfer Ability of Substituted Cyclopyrenylene Hoop-Shaped Compounds. Journal of Physical Chemistry A, 2020, 124, 3555-3563.	1.1	2
146	Some questions on the exchange contribution to the effective potential of the Kohnâ€“Sham theory. Theoretical Chemistry Accounts, 2009, 123, 197-205.	0.5	1
147	Charge generationtransport in organic materials. , 2013, , 219-244.		1
148	Morphologies and Chargeâ€Transfer: Structure and Charge Transport Properties of Cycloparaphenylene Monolayers on Graphite (Adv. Mater. Interfaces 8/2019). Advanced Materials Interfaces, 2019, 6, 1970052.	1.9	0
149	On the nature of the singlet and triplet excitations mediating thermally activated delayed fluorescence (Conference Presentation). , 2018, , .		0