

Roberto Peverati

List of Publications by Citations

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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.

47
papers

6,298
citations

21
h-index

59
g-index

59
ext. papers

7,274
ext. citations

4.4
avg, IF

6.29
L-index

#	Paper	IF	Citations
47	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015 , 113, 184-215	1.7	2068
46	Improving the Accuracy of Hybrid Meta-GGA Density Functionals by Range Separation. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 2810-2817	6.4	716
45	Quest for a universal density functional: the accuracy of density functionals across a broad spectrum of databases in chemistry and physics. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2014 , 372, 20120476	3	514
44	M11-L: A Local Density Functional That Provides Improved Accuracy for Electronic Structure Calculations in Chemistry and Physics. <i>Journal of Physical Chemistry Letters</i> , 2012 , 3, 117-124	6.4	452
43	Screened-exchange density functionals with broad accuracy for chemistry and solid-state physics. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 16187-91	3.6	409
42	An improved and broadly accurate local approximation to the exchange-correlation density functional: the MN12-L functional for electronic structure calculations in chemistry and physics. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 13171-4	3.6	277
41	Exchange-Correlation Functional with Good Accuracy for Both Structural and Energetic Properties while Depending Only on the Density and Its Gradient. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 2310-9	6.4	232
40	Communication: A global hybrid generalized gradient approximation to the exchange-correlation functional that satisfies the second-order density-gradient constraint and has broad applicability in chemistry. <i>Journal of Chemical Physics</i> , 2011 , 135, 191102	3.9	217
39	NWChem: Past, present, and future. <i>Journal of Chemical Physics</i> , 2020 , 152, 184102	3.9	187
38	Generalized Gradient Approximation That Recovers the Second-Order Density-Gradient Expansion with Optimized Across-the-Board Performance. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 1991-1997	6.4	152
37	Implementation and Performance of DFT-D with Respect to Basis Set and Functional for Study of Dispersion Interactions in Nanoscale Aromatic Hydrocarbons. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 2030-48	6.4	149
36	Performance of recent and high-performance approximate density functionals for time-dependent density functional theory calculations of valence and Rydberg electronic transition energies. <i>Journal of Chemical Physics</i> , 2012 , 137, 244104	3.9	145
35	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021 , 155, 084801	3.9	115
34	Performance of the M11 and M11-L density functionals for calculations of electronic excitation energies by adiabatic time-dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 11363-70	3.6	109
33	Blind test of density-functional-based methods on intermolecular interaction energies. <i>Journal of Chemical Physics</i> , 2016 , 145, 124105	3.9	76
32	Orbital optimized double-hybrid density functionals. <i>Journal of Chemical Physics</i> , 2013 , 139, 024110	3.9	64
31	Benchmark Database for Ylidic Bond Dissociation Energies and Its Use for Assessments of Electronic Structure Methods. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 2824-34	6.4	58

30	Density functional study of multiplicity-changing valence and Rydberg excitations of p-block elements: delta self-consistent field, collinear spin-flip time-dependent density functional theory (DFT), and conventional time-dependent DFT. <i>Journal of Chemical Physics</i> , 2011 , 135, 044118	3.9	55
29	Performance of the M11-L density functional for bandgaps and lattice constants of unary and binary semiconductors. <i>Journal of Chemical Physics</i> , 2012 , 136, 134704	3.9	54
28	The devil in the details: A tutorial review on some undervalued aspects of density functional theory calculations. <i>International Journal of Quantum Chemistry</i> , 2020 , 120, e26332	2.1	28
27	ACCCDB: A collection of chemistry databases for broad computational purposes. <i>Journal of Computational Chemistry</i> , 2019 , 40, 839-848	3.5	25
26	Assessment and validation of density functional approximations for iron carbide and iron carbide cation. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 169-73	2.8	21
25	Axial-Chiral Biisoquinoline N, N'-Dioxides Bearing Polar Aromatic C-H Bonds as Catalysts in Sakurai-Hosomi-Denmark Allylation. <i>Organic Letters</i> , 2018 , 20, 5757-5761	6.2	19
24	Hydrocarbon growth via ion-molecule reactions: computational studies of the isomers of $C_4H_2^+$, $C_4H_3^+$ and $C_4H_4^+$ and their formation paths from acetylene and its fragments. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 1859-69	3.6	17
23	What Is the Structure of the Naphthalene-Benzene Heterodimer Radical Cation? Binding Energy, Charge Delocalization, and Unexpected Charge-Transfer Interaction in Stacked Dimer and Trimer Radical Cations. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 1111-8	6.4	15
22	Statistically representative databases for density functional theory via data science. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 19092-19103	3.6	13
21	Convenient Access to Gallium(I) Cations through Hydrogen Elimination from Cationic Gallium(III) Hydrides. <i>Inorganic Chemistry</i> , 2019 , 58, 12441-12445	5.1	12
20	Ab initio quantum chemical computations of substituent effects on triaziridine strain energy and heat of formation. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 2387-95	3.6	10
19	INSIGHTS INTO HYDROCARBON CHAIN AND AROMATIC RING FORMATION IN THE INTERSTELLAR MEDIUM: COMPUTATIONAL STUDY OF THE ISOMERS OF $C_4H_3^+$, $C_6H_3^+$ AND $C_6H_5^+$ AND THEIR FORMATION	4.7	9
18	Implementation and Optimization of DFT-D/COSab with Respect to Basis Set and Functional: Application to Polar Processes of Furfural Derivatives in Solution. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 2772-86	6.4	8
17	Ozone-Induced Cleavage of Endocyclic C=C Double Bonds within Steroid Epimers Produces Unique Gas-Phase Conformations. <i>Journal of the American Society for Mass Spectrometry</i> , 2020 , 31, 411-417	3.5	7
16	Formation and stability of $C_4H_3^+$ isomers. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 10109-16	2.8	7
15	Nucleophilic Aromatic Addition in Ionizing Environments: Observation and Analysis of New C-N Valence Bonds in Complexes between Naphthalene Radical Cation and Pyridine. <i>Journal of the American Chemical Society</i> , 2017 , 139, 11923-11932	16.4	7
14	Assessment of DFT and DFT-D for Potential Energy Surfaces of Rare Gas Trimers-Implementation and Analysis of Functionals and Extrapolation Procedures. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 1951-65	6.4	7
13	Improved Identification of Isomeric Steroids Using the PaternEB̄hi Reaction with Ion Mobility-Mass Spectrometry. <i>Journal of the American Society for Mass Spectrometry</i> , 2020 , 31, 2086-2092 ^{3.5}	3.5	7

12	Spline Implementation of Generalized Gradient Approximations to the Exchange-Correlation Functional and Study of the Sensitivity of Density Functional Accuracy to Localized Domains of the Reduced Density Gradient. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 3983-94	6.4	6
11	QMC-SW: A simple workflow for quantum Monte Carlo calculations in chemistry. <i>SoftwareX</i> , 2019 , 9, 7-14	2.7	5
10	CLB18: A new structural database with unusual carbon-carbon long bonds. <i>Chemical Physics Letters</i> , 2021 , 765, 138281	2.5	5
9	Synthesis of electrophilic N-heterocyclic carbenes based on azahelicene. <i>Tetrahedron Letters</i> , 2020 , 61, 152143	2	4
8	Implementation and Performance of DFT-D with Respect to Basis Set and Functional for Study of Dispersion Interactions in Nanoscale Aromatic Hydrocarbons. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 1924	6.4	4
7	Fitting elephants in the density functionals zoo: Statistical criteria for the evaluation of density functional theory methods as a suitable replacement for counting parameters. <i>International Journal of Quantum Chemistry</i> , 2021 , 121, e26379	2.1	3
6	Competition between cyclization and unusual Norrish type I and type II nitro-acyl migration pathways in the photocaging of 1-acyl-7-nitroindoline revealed by computations. <i>Scientific Reports</i> , 2021 , 11, 1396	4.9	2
5	Design and synthesis of 3,3'-triazolyl biisoquinoline N,N'-dioxides via Hiyama cross-coupling of 4-trimethylsilyl-1,2,3-triazoles.. <i>Tetrahedron Letters</i> , 2021 , 81,	2	2
4	Evaluation of 3,3'-Triazolyl Biisoquinoline N,N'-Dioxide Catalysts for Asymmetric Hydrosilylation of Hydrazones with Trichlorosilane. <i>Catalysts</i> , 2021 , 11, 1103	4	1
3	Zinc Ammonio-dodecaborates: Synthesis, Lewis Acid Strength, and Reactivity.. <i>Inorganic Chemistry</i> , 2022 ,	5.1	1
2	A VB calculation for the excited $1\pi^+$ bound state of the H ₂ molecule. <i>Chemical Physics Letters</i> , 2006 , 417, 94-99	2.5	
1	Steps toward Rationalization of the Enantiomeric Excess of the Sakurai-Biosomi Denmark Allylation Catalyzed by Biisoquinoline N,N'-Dioxides Using Computations. <i>Catalysts</i> , 2021 , 11, 1487	4	