Roberto Peverati

List of Publications by Year
in descending order

47 papers	8,275 citations	304743 22 h-index	223800 46 g-index
59 all docs	59 docs citations	59 times ranked	7972 citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
2	Improving the Accuracy of Hybrid Meta-GGA Density Functionals by Range Separation. Journal of Physical Chemistry Letters, 2011, 2, 2810-2817.	4.6	864
3	Quest for a universal density functional: the accuracy of density functionals across a broad spectrum of databases in chemistry and physics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20120476.	3.4	599
4	M11-L: A Local Density Functional That Provides Improved Accuracy for Electronic Structure Calculations in Chemistry and Physics. Journal of Physical Chemistry Letters, 2012, 3, 117-124.	4.6	531
5	Screened-exchange density functionals with broad accuracy for chemistry and solid-state physics. Physical Chemistry Chemical Physics, 2012, 14, 16187.	2.8	525
6	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
7	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
8	An improved and broadly accurate local approximation to the exchangeâ€“correlation density functional: The MN12-L functional for electronic structure calculations in chemistry and physics. Physical Chemistry Chemical Physics, 2012, 14, 13171.	2.8	346
9	Exchangeâ€“Correlation Functional with Good Accuracy for Both Structural and Energetic Properties while Depending Only on the Density and Its Gradient. Journal of Chemical Theory and Computation, 2012, 8, 2310-2319.	5.3	276
10	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. Journal of Chemical Physics, 2011, 135, 191102.	3.0	254
11	Generalized Gradient Approximation That Recovers the Second-Order Density-Gradient Expansion with Optimized Across-the-Board Performance. Journal of Physical Chemistry Letters, 2011, 2, 1991-1997.	4.6	171
12	Performance of recent and high-performance approximate density functionals for time-dependent density functional theory calculations of valence and Rydberg electronic transition energies. Journal of Chemical Physics, 2012, 137, 244104.	3.0	165
13	Implementation and Performance of DFT-D with Respect to Basis Set and Functional for Study of Dispersion Interactions in Nanoscale Aromatic Hydrocarbons. Journal of Chemical Theory and Computation, 2008, 4, 2030-2048.	5.3	161
14	Performance of the M11 and M11-L density functionals for calculations of electronic excitation energies by adiabatic time-dependent density functional theory. Physical Chemistry Chemical Physics, 2012, 14, 11363.	2.8	154
15	Blind test of density-functional-based methods on intermolecular interaction energies. Journal of Chemical Physics, 2016, 145, 124105.	3.0	97
16	Orbital optimized double-hybrid density functionals. Journal of Chemical Physics, 2013, 139, 024110.	3.0	67
17	Performance of the M11-L density functional for bandgaps and lattice constants of unary and binary semiconductors. Journal of Chemical Physics, 2012, 136, 134704.	3.0	64
18	The devil in the details: A tutorial review on some undervalued aspects of density functional theory calculations. International Journal of Quantum Chemistry, 2020, 120, e26332.	2.0	63

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19	Benchmark Database for Ylidic Bond Dissociation Energies and Its Use for Assessments of Electronic Structure Methods. Journal of Chemical Theory and Computation, 2012, 8, 2824-2834.	5.3	62
20	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. Journal of Chemical Physics, 2011, 135, 044118.	3.0	57
21	ACCDB: A collection of chemistry databases for broad computational purposes. Journal of Computational Chemistry, 2019, 40, 839-848.	3.3	42
22	Convenient Access to Gallium(I) Cations through Hydrogen Elimination from Cationic Gallium(III) Hydrides. Inorganic Chemistry, 2019, 58, 12441-12445.	4.0	26
23	Assessment and Validation of Density Functional Approximations for Iron Carbide and Iron Carbide Cation. Journal of Physical Chemistry A, 2013, 117, 169-173.	2.5	23
24	Axial-Chiral BiisoquinolineN,Nâ€²-Dioxides Bearing Polar Aromatic C-H Bonds as Catalysts in Sakurai-Hosomi-Denmark Allylation. Organic Letters, 2018, 20, 5757-5761.	4.6	22
25	Hydrocarbon growth via ion-molecule reactions: computational studies of the isomers of C₄H₂⁺, C₆H₂⁺ and C₆H₄⁺ and their formation paths from acetylene and its fragments. Physical Chemistry Chemical Physics, 2015, 17, 1859-1869.	2.8	21
26	Statistically representative databases for density functional theory via data science. Physical Chemistry Chemical Physics, 2019, 21, 19092-19103.	2.8	20
27	What Is the Structure of the Naphthaleneâ€“Benzene Heterodimer Radical Cation? Binding Energy, Charge Delocalization, and Unexpected Charge-Transfer Interaction in Stacked Dimer and Trimer Radical Cations. Journal of Physical Chemistry Letters, 2015, 6, 1111-1118.	4.6	16
28	Improved Identification of Isomeric Steroids Using the PaternÃ²-BÃ¼chi Reaction with Ion Mobility-Mass Spectrometry. Journal of the American Society for Mass Spectrometry, 2020, 31, 2086-2092.	2.8	14
29	Ab initio quantum chemical computations of substituent effects on triaziridine strain energy and heat of formation. Physical Chemistry Chemical Physics, 2009, 11, 2387.	2.8	11
30	INSIGHTS INTO HYDROCARBON CHAIN AND AROMATIC RING FORMATION IN THE INTERSTELLAR MEDIUM: COMPUTATIONAL STUDY OF THE ISOMERS OF AND AND THEIR FORMATION PATHWAYS. Astrophysical Journal, 2016, 830, 128.	4.5	11
31	Nucleophilic Aromatic Addition in Ionizing Environments: Observation and Analysis of New Câ€“N Valence Bonds in Complexes between Naphthalene Radical Cation and Pyridine. Journal of the American Chemical Society, 2017, 139, 11923-11932.	13.7	11
32	CLB18: A new structural database with unusual carbonâ€“carbon long bonds. Chemical Physics Letters, 2021, 765, 138281.	2.6	11
33	Implementation and Optimization of DFT-D/COSab with Respect to Basis Set and Functional: Application to Polar Processes of Furfural Derivatives in Solution. Journal of Chemical Theory and Computation, 2009, 5, 2772-2786.	5.3	9
34	Ozone-Induced Cleavage of Endocyclic Câ•C Double Bonds within Steroid Epimers Produces Unique Gas-Phase Conformations. Journal of the American Society for Mass Spectrometry, 2020, 31, 411-417.	2.8	9
35	Assessment of DFT and DFT-D for Potential Energy Surfaces of Rare Gas Trimersâ€”Implementation and Analysis of Functionals and Extrapolation Procedures. Journal of Chemical Theory and Computation, 2010, 6, 1951-1965.	5.3	8
36	Formation and Stability of C₆H₃⁺ Isomers. Journal of Physical Chemistry A, 2014, 118, 10109-10116.	2.5	8

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37	Synthesis of electrophilic N-heterocyclic carbenes based on azahelicene. Tetrahedron Letters, 2020, 61, 152143.	1.4	7
38	Fitting elephants in the density functionals zoo: Statistical criteria for the evaluation of density functional theory methods as a suitable replacement for counting parameters. International Journal of Quantum Chemistry, 2021, 121, e26379.	2.0	7
39	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. Journal of Chemical Theory and Computation, 2011, 7, 3983-3994.	5.3	6
40	QMC-SW: A simple workflow for quantum Monte Carlo calculations in chemistry. SoftwareX, 2019, 9, 7-14.	2.6	6
41	Zinc Ammonio-dodecaborates: Synthesis, Lewis Acid Strength, and Reactivity. Inorganic Chemistry, 2022, 61, 7032-7042.	4.0	6
42	Implementation and Performance of DFT-D with Respect to Basis Set and Functional for Study of Dispersion Interactions in Nanoscale Aromatic Hydrocarbons. Journal of Chemical Theory and Computation, 2010, 6, 1924-1924.	5.3	4
43	Competition between cyclization and unusual Norrish type I and type II nitro-acyl migration pathways in the photouncaging of 1-acyl-7-nitroindoline revealed by computations. Scientific Reports, 2021, 11, 1396.	3.3	4
44	Evaluation of 3,3â€²-Triazolyl Biisoquinoline N,Nâ€²-Dioxide Catalysts for Asymmetric Hydrosilylation of Hydrazones with Trichlorosilane. Catalysts, 2021, 11, 1103.	3.5	4
45	Design and synthesis of 3,3â€²-triazolyl biisoquinoline N,Nâ€™-dioxides via Hiyama cross-coupling of 4-trimethylsilyl-1,2,3-triazoles. Tetrahedron Letters, 2021, 81, 153338.	1.4	4
46	A VB calculation for the excited <mml:math altimg="si9.gif" display="inline" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http:/. Chemical Physics Let.	2.6	0
47	Steps toward Rationalization of the Enantiomeric Excess of the Sakuraiâ€“Hosomiâ€“Denmark Allylation Catalyzed by Biisoquinoline N,Nâ€™-Dioxides Using Computations. Catalysts, 2021, 11, 1487.	3.5	0