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	Zinc Ammonio-dodecaborates: Synthesis, Lewis Acid Strength, and Reactivity. Inorganic Chemistry, 2022, 61, 7032-7042.	4.0	6
2	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
3	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
4	CLB18: A new structural database with unusual carbonâ€“carbon long bonds. Chemical Physics Letters, 2021, 765, 138281.	2.6	11
5	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
6	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
7	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
8	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
9	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
10	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
11	Synthesis of electrophilic N-heterocyclic carbenes based on azahelicene. Tetrahedron Letters, 2020, 61, 152143.	1.4	7
12	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
13	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
14	Statistically representative databases for density functional theory via data science. Physical Chemistry Chemical Physics, 2019, 21, 19092-19103.	2.8	20
15	Convenient Access to Gallium(I) Cations through Hydrogen Elimination from Cationic Gallium(III) Hydrides. Inorganic Chemistry, 2019, 58, 12441-12445.	4.0	26
16	ACCDB: A collection of chemistry databases for broad computational purposes. Journal of Computational Chemistry, 2019, 40, 839-848.	3.3	42
17	QMC-SW: A simple workflow for quantum Monte Carlo calculations in chemistry. SoftwareX, 2019, 9, 7-14.	2.6	6
18	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

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19	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
20	Blind test of density-functional-based methods on intermolecular interaction energies. Journal of Chemical Physics, 2016, 145, 124105.	3.0	97
21	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
22	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
23	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
24	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
25	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
26	Formation and Stability of C₆H₃⁺ Isomers. Journal of Physical Chemistry A, 2014, 118, 10109-10116.	2.5	8
27	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
28	Orbital optimized double-hybrid density functionals. Journal of Chemical Physics, 2013, 139, 024110.	3.0	67
29	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
30	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
31	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
32	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
33	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
34	Screened-exchange density functionals with broad accuracy for chemistry and solid-state physics. Physical Chemistry Chemical Physics, 2012, 14, 16187.	2.8	525
35	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
36	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

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37	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
38	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
39	Improving the Accuracy of Hybrid Meta-GGA Density Functionals by Range Separation. Journal of Physical Chemistry Letters, 2011, 2, 2810-2817.	4.6	864
40	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
41	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
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	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
44	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
45	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
46	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
47	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"	2.6	0