Roberto Peverati

List of Publications by Year in Descending Order

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	Zinc Ammonio-dodecaborates: Synthesis, Lewis Acid Strength, and Reactivity.. *Inorganic Chemistry*, **2022**,	5.1	1
46	Steps toward Rationalization of the Enantiomeric Excess of the Sakurai–Hosomi–Denmark Allylation Catalyzed by Biisoquinoline N,N′-Dioxides Using Computations. *Catalysts*, **2021**, 11, 1487	4	
45	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	2.1	3
44	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	4.9	2
43	CLB18: A new structural database with unusual carbon–carbon long bonds. *Chemical Physics Letters*, **2021**, 765, 138281	2.5	5
42	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
41	Evaluation of 3,3?-Triazolyl Biisoquinoline N,N?-Dioxide Catalysts for Asymmetric Hydrosilylation of Hydrazones with Trichlorosilane. *Catalysts*, **2021**, 11, 1103	4	1
40	Design and synthesis of 3,3'-triazolyl biisoquinoline ,-dioxides via Hiyama cross-coupling of 4-trimethylsilyl-1,2,3-triazoles.. *Tetrahedron Letters*, **2021**, 81,	2	2
39	NWChem: Past, present, and future. *Journal of Chemical Physics*, **2020**, 152, 184102	3.9	187
38	Synthesis of electrophilic N-heterocyclic carbenes based on azahelicene. *Tetrahedron Letters*, **2020**, 61, 152143	2	4
37	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	2.1	28
36	Ozone-Induced Cleavage of Endocyclic C?C Double Bonds within Steroid Epimers Produces Unique Gas-Phase Conformations. *Journal of the American Society for Mass Spectrometry*, **2020**, 31, 411-417	3.5	7
35	Improved Identification of Isomeric Steroids Using the Paternò–Büchi Reaction with Ion Mobility-Mass Spectrometry. *Journal of the American Society for Mass Spectrometry*, **2020**, 31, 2086-2092	3.5	7
34	Convenient Access to Gallium(I) Cations through Hydrogen Elimination from Cationic Gallium(III) Hydrides. *Inorganic Chemistry*, **2019**, 58, 12441-12445	5.1	12
33	Statistically representative databases for density functional theory via data science. *Physical Chemistry Chemical Physics*, **2019**, 21, 19092-19103	3.6	13
32	ACCDB: A collection of chemistry databases for broad computational purposes. *Journal of Computational Chemistry*, **2019**, 40, 839-848	3.5	25
31	QMC-SW: A simple workflow for quantum Monte Carlo calculations in chemistry. *SoftwareX*, **2019**, 9, 7-14	2.7	5

30	Axial-Chiral Biisoquinoline N, N'-Dioxides Bearing Polar Aromatic C-H Bonds as Catalysts in Sakurai-Hosomi-Denmark Allylation. *Organic Letters*, **2018**, 20, 5757-5761	6.2	19
29	Nucleophilic Aromatic Addition in Ionizing Environments: Observation and Analysis of New C-N Valence Bonds in Complexes between Naphthalene Radical Cation and Pyridine. *Journal of the American Chemical Society*, **2017**, 139, 11923-11932	16.4	7
28	INSIGHTS INTO HYDROCARBON CHAIN AND AROMATIC RING FORMATION IN THE INTERSTELLAR MEDIUM: COMPUTATIONAL STUDY OF THE ISOMERS OF ${{rm{C}}}_{4}{{{rm{H}}}_{3}}^{+}$ ${{rm{C}}}_{6}{{{rm{H}}}_{3}}^{+}$ AND ${{rm{C}}}_{6}{{{rm{H}}}_{5}}^{+}$ AND THEIR FORMATION PATHWAYS. *Astrophysical Journal*, **2016**, 830, 128	4.7	9
27	Blind test of density-functional-based methods on intermolecular interaction energies. *Journal of Chemical Physics*, **2016**, 145, 124105	3.9	76
26	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. *Journal of Physical Chemistry Letters*, **2015**, 6, 1111-8	6.4	15
25	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
24	Hydrocarbon growth via ion-molecule reactions: computational studies of the isomers of CH2+, CH+ and CH+ and their formation paths from acetylene and its fragments. *Physical Chemistry Chemical Physics*, **2015**, 17, 1859-69	3.6	17
23	Formation and stability of CH+ isomers. *Journal of Physical Chemistry A*, **2014**, 118, 10109-16	2.8	7
22	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	514
21	Assessment and validation of density functional approximations for iron carbide and iron carbide cation. *Journal of Physical Chemistry A*, **2013**, 117, 169-73	2.8	21
20	Orbital optimized double-hybrid density functionals. *Journal of Chemical Physics*, **2013**, 139, 024110	3.9	64
19	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	3.9	145
18	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	6.4	452
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	3.9	54
16	Benchmark Database for Ylidic Bond Dissociation Energies and Its Use for Assessments of Electronic Structure Methods. *Journal of Chemical Theory and Computation*, **2012**, 8, 2824-34	6.4	58
15	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. *Physical Chemistry Chemical Physics*, **2012**, 14, 13171-4	3.6	277
14	Screened-exchange density functionals with broad accuracy for chemistry and solid-state physics. *Physical Chemistry Chemical Physics*, **2012**, 14, 16187-91	3.6	409
13	Exchange-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, 2310-9	6.4	232

12	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, 11363-70	3.6	109
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	6.4	152
10	Improving the Accuracy of Hybrid Meta-GGA Density Functionals by Range Separation. *Journal of Physical Chemistry Letters*, **2011**, 2, 2810-2817	6.4	716
9	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, 3983-94	6.4	6
8	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	3.9	55
7	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	3.9	217
6	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	6.4	4
5	Assessment of DFT and DFT-D for Potential Energy Surfaces of Rare Gas Trimers-Implementation and Analysis of Functionals and Extrapolation Procedures. *Journal of Chemical Theory and Computation*, **2010**, 6, 1951-65	6.4	7
4	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, 2772-86	6.4	8
3	Ab initio quantum chemical computations of substituent effects on triaziridine strain energy and heat of formation. *Physical Chemistry Chemical Physics*, **2009**, 11, 2387-95	3.6	10
2	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, 2030-48	6.4	149
1	A VB calculation for the excited 1Σ+ bound state of the H2 molecule. *Chemical Physics Letters*, **2006**, 417, 94-99	2.5	