

Juan E Peralta

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/8545624/publications.pdf>

Version: 2024-02-01

102
papers

6,496
citations

109137

35
h-index

62479

80
g-index

104
all docs

104
docs citations

104
times ranked

6754
citing authors

#	ARTICLE	IF	CITATIONS
1	Energy band gaps and lattice parameters evaluated with the Heyd-Scuseria-Ernzerhof screened hybrid functional. <i>Journal of Chemical Physics</i> , 2005, 123, 174101.	1.2	1,604
2	Enhanced Half-Metallicity in Edge-Oxidized Zigzag Graphene Nanoribbons. <i>Nano Letters</i> , 2007, 7, 2295-2299.	4.5	547
3	Magnetic Boron Nitride Nanoribbons with Tunable Electronic Properties. <i>Nano Letters</i> , 2008, 8, 2210-2214.	4.5	317
4	Angular dependence of spin-spin coupling constants. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2000, 37, 321-425.	3.9	286
5	Spin-orbit splittings and energy band gaps calculated with the Heyd-Scuseria-Ernzerhof screened hybrid functional. <i>Physical Review B</i> , 2006, 74, .	1.1	182
6	Basis set dependence of NMR spin-spin couplings in density functional theory calculations: first row and hydrogen atoms. <i>Chemical Physics Letters</i> , 2003, 375, 452-458.	1.2	179
7	Edge effects in finite elongated graphene nanoribbons. <i>Physical Review B</i> , 2007, 76, .	1.1	148
8	DFT Calculation of NMR Spin-Spin Coupling Constants in Fluorinated Pyridines. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5607-5612.	1.1	146
9	Electronic Properties of the Biphenylene Sheet and Its One-Dimensional Derivatives. <i>ACS Nano</i> , 2010, 4, 4565-4570.	7.3	124
10	Lithium adsorption on zigzag graphene nanoribbons. <i>Journal of Applied Physics</i> , 2009, 106, .	1.1	117
11	Accurate Prediction of the Electronic Properties of Low-Dimensional Graphene Derivatives Using a Screened Hybrid Density Functional. <i>Accounts of Chemical Research</i> , 2011, 44, 269-279.	7.6	115
12	Machine Learning the Voltage of Electrode Materials in Metal-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 18494-18503.	4.0	104
13	Substituent Effects on Scalar $2J(19F,19F)$ and $3J(19F,19F)$ NMR Couplings: A Comparison of SOPPA and DFT Methods. <i>Journal of Physical Chemistry A</i> , 2003, 107, 4748-4754.	1.1	103
14	Advances in Theoretical and Physical Aspects of Spin-Spin Coupling Constants. <i>Annual Reports on NMR Spectroscopy</i> , 2003, 51, 167-260.	0.7	102
15	Advances in theoretical and physical aspects of spin-spin coupling constants. <i>Annual Reports on NMR Spectroscopy</i> , 2000, 41, 55-184.	0.7	100
16	Hexagonal BC ₃ : A Robust Electrode Material for Li, Na, and K Ion Batteries. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2728-2732.	2.1	100
17	Density functional investigations of the properties and thermochemistry of UF ₆ and UF ₅ using valence-electron and all-electron approaches. <i>Journal of Chemical Physics</i> , 2004, 121, 2144-2150.	1.2	93
18	Density Functional Theory Study of Optical Transitions in Semiconducting Single-Walled Carbon Nanotubes. <i>Nano Letters</i> , 2005, 5, 1621-1624.	4.5	92

#	ARTICLE	IF	CITATIONS
19	Through-Bond and Through-Space ^1H - ^1H Spin-Spin Coupling in Perdifluoronaphthalenes: Accurate DFT Evaluation of the Four Contributions. <i>Journal of the American Chemical Society</i> , 2001, 123, 9162-9163.	6.6	88
20	Screened exchange hybrid density-functional study of the work function of pristine and doped single-walled carbon nanotubes. <i>Journal of Chemical Physics</i> , 2006, 124, 024709.	1.2	87
21	Noncollinear magnetism in density functional calculations. <i>Physical Review B</i> , 2007, 75, .	1.1	83
22	Non-empirical calculations of NMR indirect carbon-carbon coupling constants: 1. Three-membered rings. <i>Magnetic Resonance in Chemistry</i> , 2002, 40, 187-194.	1.1	69
23	Optical Transitions in Metallic Single-Walled Carbon Nanotubes. <i>Nano Letters</i> , 2005, 5, 1830-1833.	4.5	66
24	Assessment of Density Functionals for Predicting One-Bond Carbon-Hydrogen NMR Spin-Spin Coupling Constants. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 541-545.	2.3	66
25	Dispersion in the Mott insulator UO_2 : A comparison of photoemission spectroscopy and screened hybrid density functional theory. <i>Journal of Computational Chemistry</i> , 2008, 29, 2288-2294.	1.5	65
26	Relativistic all-electron two-component self-consistent density functional calculations including one-electron scalar and spin-orbit effects. <i>Journal of Chemical Physics</i> , 2004, 120, 5875-5881.	1.2	62
27	Basis set dependence of atomic spin populations. <i>Chemical Physics Letters</i> , 2010, 495, 146-150.	1.2	62
28	Self-interaction error overbinds water clusters but cancels in structural energy differences. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 11283-11288.	3.3	57
29	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. <i>Journal of Chemical Physics</i> , 2019, 151, 214108.	1.2	56
30	Natural coupling (NJC) analysis of the electron lone pair effect on NMR couplings: Part 1. The lone pair orientation effect of an α -nitrogen atom on $^1\text{J}(\text{C},\text{C})$ couplings. <i>Magnetic Resonance in Chemistry</i> , 2001, 39, 600-606.	1.1	54
31	Magnetic Exchange Couplings with Range-Separated Hybrid Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1894-1899.	2.3	53
32	Stretched or noded orbital densities and self-interaction correction in density functional theory. <i>Journal of Chemical Physics</i> , 2019, 150, 174102.	1.2	46
33	Relativistic calculation of indirect NMR spin-spin couplings using the Douglas-Kroll-Hess approximation. <i>Journal of Chemical Physics</i> , 2005, 123, 204112.	1.2	45
34	The role of range-separated Hartree-Fock exchange in the calculation of magnetic exchange couplings in transition metal complexes. <i>Journal of Chemical Physics</i> , 2011, 134, 034108.	1.2	37
35	All-Electron Hybrid Density Functional Calculations on UF_n and UCln ($n = 1\text{--}6$). <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 612-616.	2.3	36
36	Density functional theory study of bulk platinum monoxide. <i>Physical Review B</i> , 2005, 71, .	1.1	34

#	ARTICLE	IF	CITATIONS
37	Magnetic Exchange Couplings from Semilocal Functionals Evaluated Nonself-Consistently on Hybrid Densities: Insights on Relative Importance of Exchange, Correlation, and Delocalization. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3147-3158.	2.3	34
38	First-principles electronic transport calculations in finite elongated systems: A divide and conquer approach. <i>Journal of Chemical Physics</i> , 2006, 125, 114704.	1.2	33
39	Fermi-LÅrdin orbital self-interaction correction to magnetic exchange couplings. <i>Journal of Chemical Physics</i> , 2018, 149, 164101.	1.2	33
40	Natural coupling (NJC) analysis of the electron lone pair effect on NMR couplings: 2. The anomeric effects on J(C, H) couplings and its dependence on solvent. <i>Molecular Physics</i> , 2002, 100, 705-715.	0.8	32
41	Anomeric Effect on Geminal and Vicinal H NMR Coupling Constants. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7762-7768.	1.1	31
42	Towards the blackbox computation of magnetic exchange coupling parameters in polynuclear transition-metal complexes: Theory, implementation, and application. <i>Journal of Chemical Physics</i> , 2013, 138, 174115.	1.2	31
43	Shrinking Self-Interaction Errors with the Fermi-LÅrdin Orbital Self-Interaction-Corrected Density Functional Approximation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9307-9315.	1.1	30
44	The effect of self-interaction error on electrostatic dipoles calculated using density functional theory. <i>Journal of Chemical Physics</i> , 2019, 151, 174106.	1.2	29
45	Scalar relativistic all-electron density functional calculations on periodic systems. <i>Journal of Chemical Physics</i> , 2005, 122, 084108.	1.2	28
46	Magnetization Dynamics from Time-Dependent Noncollinear Spin Density Functional Theory Calculations. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3661-3668.	2.3	28
47	DFT-GIAO and DFT-NBO studies of the origin of ¹⁹ F NMR shielding effects in alkyl fluorides. <i>Magnetic Resonance in Chemistry</i> , 1999, 37, 167-172.	1.1	27
48	Self-interaction-free electric dipole polarizabilities for atoms and their ions using the Fermi-LÅrdin self-interaction correction. <i>Physical Review A</i> , 2019, 100, .	1.0	27
49	Finite perturbation theory-density functional theory calculation of the spin-dipolar contribution to NMR spin-spin coupling constants. <i>Molecular Physics</i> , 2001, 99, 655-661.	0.8	26
50	Density Functional Theory Calculation of Indirect Nuclear Magnetic Resonance Spin-Spin Coupling Constants in C70. <i>Journal of the American Chemical Society</i> , 2004, 126, 7428-7429.	6.6	26
51	Vicinal NMR Proton-Proton Coupling Constants. An NBO Analysis. <i>Journal of Physical Chemistry A</i> , 2001, 105, 5298-5303.	1.1	25
52	On the Capriciousness of the FCCF Karplus Curve. <i>Journal of the American Chemical Society</i> , 2002, 124, 9702-9703.	6.6	25
53	Magnetic exchange couplings from noncollinear spin density functional perturbation theory. <i>Journal of Chemical Physics</i> , 2008, 129, 194107.	1.2	24
54	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. II. Gauge consistency of the energy density at three levels of approximation. <i>Journal of Chemical Physics</i> , 2020, 152, 214109.	1.2	23

#	ARTICLE	IF	CITATIONS
55	On the Question of the Total Energy in the Fermiâ€“LÃ¡wdin Orbital Self-Interaction Correction Method. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4122-4128.	2.3	22
56	Natural bond orbitals analysis of Câ€“Hâ€“O interactions in NCH/H 2 O and NCH/OCH 2 , and their effect on nuclear magnetic shielding constants. <i>Computational and Theoretical Chemistry</i> , 1999, 491, 23-31.	1.5	21
57	Solvent Effects on Nuclear Magnetic Resonance 2J(C,Hf) and 1J(C,Hf) Spinâ€“Spin Coupling Constants in Acetaldehyde. <i>International Journal of Molecular Sciences</i> , 2003, 4, 93-106.	1.8	21
58	Interpretation and Automatic Generation of Fermiâ€“Orbital Descriptors. <i>Journal of Computational Chemistry</i> , 2019, 40, 2843-2857.	1.5	21
59	A DFT/GIAO/NBO and experimental study of 13C SCSs in 1-X-bicyclo[1.1.1]pentanes. <i>Magnetic Resonance in Chemistry</i> , 2000, 38, 395-402.	1.1	20
60	NMR3J(C1,H3) couplings in 1-X-bicyclo[1.1.1]pentanes. FPT-DFT and NBO studies of hyperconjugative interactions and heavy atom substituent effects. <i>Journal of Computational Chemistry</i> , 2001, 22, 1615-1621.	1.5	20
61	Theoretical study of charge transfer interactions in methanol adsorbed on magnesium oxide. <i>Surface Science</i> , 2002, 504, 235-243.	0.8	19
62	Computation and analysis of 19F substituent chemical shifts of some bridgehead-substituted polycyclic alkyl fluorides. <i>Magnetic Resonance in Chemistry</i> , 2003, 41, 503-508.	1.1	18
63	Magnetic exchange couplings from constrained density functional theory: An efficient approach utilizing analytic derivatives. <i>Journal of Chemical Physics</i> , 2011, 135, 184108.	1.2	18
64	Accuracy of density functional theory methods for the calculation of magnetic exchange couplings in binuclear iron(III) complexes. <i>Polyhedron</i> , 2020, 176, 114194.	1.0	18
65	Prediction of vicinal protonâ€“proton coupling constants $\langle \sup 3 \rangle \langle i \rangle \langle \sub HH \rangle$ from density functional theory calculations. <i>Molecular Physics</i> , 2005, 103, 1307-1326.	0.8	16
66	Analytic atomic gradients in the fermiâ€“LÃ¡wdin orbital selfâ€“interaction correction. <i>Journal of Computational Chemistry</i> , 2019, 40, 820-825.	1.5	16
67	Magnetic exchange couplings evaluated with Rung 3.5 density functionals. <i>Journal of Chemical Physics</i> , 2011, 134, 214101.	1.2	14
68	Magnetic Couplings in Spin Frustrated Fe7III Disklike Clusters. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5585-5589.	2.3	14
69	Magnetic Properties of Mononuclear Co(II) Complexes with Carborane Ligands. <i>Inorganic Chemistry</i> , 2018, 57, 7763-7769.	1.9	14
70	How well do self-interaction corrections repair the overestimation of static polarizabilities in density functional calculations?. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18678-18685.	1.3	14
71	Structural dependence of magnetic exchange coupling parameters in transition-metal complexes. <i>Chemical Physics Letters</i> , 2013, 557, 110-113.	1.2	13
72	Magnetic Exchange Couplings in Heterodinuclear Complexes Based on Differential Local Spin Rotations. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1728-1734.	2.3	13

#	ARTICLE	IF	CITATIONS
73	On the convergence of FPT-DFT calculations of the Fermi contact contribution to NMR coupling constants. <i>Theoretical Chemistry Accounts</i> , 2000, 105, 165-168.	0.5	12
74	Intramolecular electric field effect on a1J(C,H) NMR spin-spin coupling constant. an experimental and theoretical study. <i>Magnetic Resonance in Chemistry</i> , 1999, 37, 227-231.	1.1	11
75	Graphene Nanoribbons-Based Ultrasensitive Chemical Detectors. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3791-3797.	1.5	11
76	Magnetic Properties of Co(II) Complexes with Polyhedral Carborane Ligands. <i>Inorganic Chemistry</i> , 2019, 58, 2550-2557.	1.9	11
77	Magnetic Exchange Couplings from Noncollinear Perturbation Theory: Dinuclear Cu ^{II} Complexes. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5841-5847.	1.1	10
78	Iron(III)â€“Oxo Cluster Chemistry with Dimethylarsinate Ligands: Structures, Magnetic Properties, and Computational Studies. <i>Inorganic Chemistry</i> , 2020, 59, 18090-18101.	1.9	10
79	Density-related properties from self-interaction corrected density functional theory calculations. <i>Journal of Chemical Physics</i> , 2021, 154, 024102.	1.2	8
80	Gradient copolymers of thiophene and pyrrole for photovoltaics. <i>Computational Materials Science</i> , 2015, 96, 69-71.	1.4	7
81	Local Noncollinear Spin Analysis. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6101-6107.	2.3	7
82	Atomic structure and Mott nature of the insulating charge density wave phase of 1T-TaS ₂ . <i>Journal of Physics Condensed Matter</i> , 2022, 34, 345401.	0.7	7
83	Study of Self-Interaction Errors in Density Functional Calculations of Magnetic Exchange Coupling Constants Using Three Self-Interaction Correction Methods. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1923-1935.	1.1	6
84	Substituent effects on scalarJ(13C,13C) couplings in pyrimidines. An experimental and DFT study. <i>Magnetic Resonance in Chemistry</i> , 2004, 42, 938-943.	1.1	5
85	Molecular spin frustration in mixed-chelate Fe ⁵ and Fe ⁶ oxo clusters with high ground state spin values. <i>Polyhedron</i> , 2020, 176, 114182.	1.0	5
86	Magnetic Properties of High-Nuclearity Fe ^x -oxo (x = 7, 22, 24) Clusters Analyzed by a Multipronged Experimental, Computational, and Magnetostructural Correlation Approach. <i>Inorganic Chemistry</i> , 0, , .	1.9	5
87	A simple spectrophotometric method to determine phytic acid in poultry wastewater without acid digestion. <i>International Journal of Environmental Analytical Chemistry</i> , 2020, , 1-11.	1.8	4
88	Initial Fermi orbital descriptors for FLOSIC calculations: The quick-FOD method. <i>Chemical Physics Letters</i> , 2021, 780, 138952.	1.2	4
89	Magnetic control over the fundamental structure of atomic wires. <i>Nature Communications</i> , 2022, 13, .	5.8	4
90	Electrostatic effect of the polar bond-polarizable bond interaction on13C chemical shifts. <i>International Journal of Quantum Chemistry</i> , 1998, 70, 105-112.	1.0	3

#	ARTICLE	IF	CITATIONS
91	The polar bondâ€“polarizable bond interaction in 1-X,2-methoxy naphthalenes. An experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2000, 556, 263-273.	1.8	3
92	Theoretical NMR $J(13C,13C)$ Scalar Couplings as Probes to Study Diamagnetic Ring Currents in Fullerenes. <i>Advances in Quantum Chemistry</i> , 2005, , 127-139.	0.4	3
93	The performance of density functional approximations for the structures and relative energies of minimum energy crossing points. <i>Chemical Physics Letters</i> , 2013, 590, 227-230.	1.2	3
94	Modeling of Quasi-One-Dimensional Carbon Nanostructures with Density Functional Theory. , 2012, , 901-938.		2
95	Magnetic properties of closo-carborane-based Co(II) single-ion complexes with O, S, Se, and Te bridging atoms. <i>Polyhedron</i> , 2020, 176, 114257.	1.0	2
96	Fermiâ€“LÃ“wdin orbital self-interaction correction of adsorption energies on transition metal ions. <i>Journal of Chemical Physics</i> , 2022, 156, 134102.	1.2	2
97	Comment on â€œAdditional Insights Between Fermiâ€“LÃ“wdin Orbital SIC and the Localization Equation Constraints in SIC-DFTâ€“, <i>Journal of Physical Chemistry A</i> , 2019, 123, 4322-4323.	1.1	1
98	Analysis of spin frustration in an FeIII7 cluster using a combination of computational, experimental, and magnetostructural correlation methods. <i>Polyhedron</i> , 2022, 225, 116045.	1.0	1
99	Advances in Theoretical and Physical Aspects of Spinâ€“Spin Coupling Constants. <i>ChemInform</i> , 2005, 36, no.	0.1	0
100	Site-specific polarizabilities from analytic linear-response theory. <i>Chemical Physics Letters</i> , 2014, 608, 24-27.	1.2	0
101	Modeling of Quasi-One-Dimensional Carbon Nanostructures with Density Functional Theory. , 2017, , 1297-1337.		0
102	Modeling of Quasi-One-Dimensional Carbon Nanostructures with Density Functional Theory. , 2015, , 1-41.		0