Juan E Peralta

List of Publications by Year in descending order

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102	6,496	109264	62565
papers	citations	35 h-index	80 g-index

104	104	104	6754
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Energy band gaps and lattice parameters evaluated with the Heyd-Scuseria-Ernzerhof screened hybrid functional. Journal of Chemical Physics, 2005, 123, 174101.	1.2	1,604
2	Enhanced Half-Metallicity in Edge-Oxidized Zigzag Graphene Nanoribbons. Nano Letters, 2007, 7, 2295-2299.	4.5	547
3	Magnetic Boron Nitride Nanoribbons with Tunable Electronic Properties. Nano Letters, 2008, 8, 2210-2214.	4.5	317
4	Angular dependence of spinâ€“spin coupling constants. Progress in Nuclear Magnetic Resonance Spectroscopy, 2000, 37, 321-425.	3.9	286
5	Spin-orbit splittings and energy band gaps calculated with the Heyd-Scuseria-Ernzerhof screened hybrid functional. Physical Review B, 2006, 74, .	1.1	182
6	Basis set dependence of NMR spinâ€“spin couplings in density functional theory calculations: first row and hydrogen atoms. Chemical Physics Letters, 2003, 375, 452-458.	1.2	179
7	Edge effects in finite elongated graphene nanoribbons. Physical Review B, 2007, 76, .	1.1	148
8	DFT Calculation of NMRJFFSpinâ^'Spin Coupling Constants in Fluorinated Pyridines. Journal of Physical Chemistry A, 2002, 106, 5607-5612.	1.1	146
9	Electronic Properties of the Biphenylene Sheet and Its One-Dimensional Derivatives. ACS Nano, 2010, 4, 4565-4570.	7.3	124
10	Lithium adsorption on zigzag graphene nanoribbons. Journal of Applied Physics, 2009, 106, .	1.1	117
11	Accurate Prediction of the Electronic Properties of Low-Dimensional Graphene Derivatives Using a Screened Hybrid Density Functional. Accounts of Chemical Research, 2011, 44, 269-279.	7.6	115
12	Machine Learning the Voltage of Electrode Materials in Metal-Ion Batteries. ACS Applied Materials & Interfaces, 2019, 11, 18494-18503.	4.0	104
13	Substituent Effects on Scalar 2J(19F,19F) and 3J(19F,19F) NMR Couplings:â€‰ A Comparison of SOPPA and DFT Methods. Journal of Physical Chemistry A, 2003, 107, 4748-4754.	1.1	103
14	Advances in Theoretical and Physical Aspects of Spinâ€“Spin Coupling Constants. Annual Reports on NMR Spectroscopy, 2003, 51, 167-260.	0.7	102
15	Advances in theoretical and physical aspects of spin-spin coupling constants. Annual Reports on NMR Spectroscopy, 2000, 41, 55-184.	0.7	100
16	Hexagonal BC₃: A Robust Electrode Material for Li, Na, and K Ion Batteries. Journal of Physical Chemistry Letters, 2015, 6, 2728-2732.	2.1	100
17	Density functional investigations of the properties and thermochemistry of UF6 and UF5 using valence-electron and all-electron approaches. Journal of Chemical Physics, 2004, 121, 2144-2150.	1.2	93
18	Density Functional Theory Study of Optical Transitions in Semiconducting Single-Walled Carbon Nanotubes. Nano Letters, 2005, 5, 1621-1624.	4.5	92

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19	Through-Bond and Through-SpaceJFFSpinâ^'Spin Coupling in Peridifluoronaphthalenes:Â Accurate DFT Evaluation of the Four Contributions. Journal of the American Chemical Society, 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. Journal of Chemical Physics, 2006, 124, 024709.	1.2	87
21	Noncollinear magnetism in density functional calculations. Physical Review B, 2007, 75, .	1.1	83
22	Non-empirical calculations of NMR indirect carbon-carbon coupling constants: 1. Three-membered rings. Magnetic Resonance in Chemistry, 2002, 40, 187-194.	1.1	69
23	Optical Transitions in Metallic Single-Walled Carbon Nanotubes. Nano Letters, 2005, 5, 1830-1833.	4.5	66
24	Assessment of Density Functionals for Predicting One-Bond Carbonâ^'Hydrogen NMR Spinâ^'Spin Coupling Constants. Journal of Chemical Theory and Computation, 2005, 1, 541-545.	2.3	66
25	Dispersion in the Mott insulator UO₂: A comparison of photoemission spectroscopy and screened hybrid density functional theory. Journal of Computational Chemistry, 2008, 29, 2288-2294.	1.5	65
26	Relativistic all-electron two-component self-consistent density functional calculations including one-electron scalar and spinâ€“orbit effects. Journal of Chemical Physics, 2004, 120, 5875-5881.	1.2	62
27	Basis set dependence of atomic spin populations. Chemical Physics Letters, 2010, 495, 146-150.	1.2	62
28	Self-interaction error overbinds water clusters but cancels in structural energy differences. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 11283-11288.	3.3	57
29	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. Journal of Chemical Physics, 2019, 151, 214108.	1.2	56
30	NaturalJ coupling (NJC) analysis of the electron lone pair effect on NMR couplings: Part 1. The lone pair orientation effect of an ?-nitrogen atom on1J(C,C) couplings. Magnetic Resonance in Chemistry, 2001, 39, 600-606.	1.1	54
31	Magnetic Exchange Couplings with Range-Separated Hybrid Density Functionals. Journal of Chemical Theory and Computation, 2010, 6, 1894-1899.	2.3	53
32	Stretched or noded orbital densities and self-interaction correction in density functional theory. Journal of Chemical Physics, 2019, 150, 174102.	1.2	46
33	Relativistic calculation of indirect NMR spin-spin couplings using the Douglas-Kroll-Hess approximation. Journal of Chemical Physics, 2005, 123, 204112.	1.2	45
34	The role of range-separated Hartreeâ€“Fock exchange in the calculation of magnetic exchange couplings in transition metal complexes. Journal of Chemical Physics, 2011, 134, 034108.	1.2	37
35	All-Electron Hybrid Density Functional Calculations on UFn and UCln (n = 1â^'6). Journal of Chemical Theory and Computation, 2005, 1, 612-616.	2.3	36
36	Density functional theory study of bulk platinum monoxide. Physical Review B, 2005, 71, .	1.1	34

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37	Magnetic Exchange Couplings from Semilocal Functionals Evaluated Nonself-Consistently on Hybrid Densities: Insights on Relative Importance of Exchange, Correlation, and Delocalization. Journal of Chemical Theory and Computation, 2012, 8, 3147-3158.	2.3	34
38	First-principles electronic transport calculations in finite elongated systems: A divide and conquer approach. Journal of Chemical Physics, 2006, 125, 114704.	1.2	33
39	Fermi-LÃ¶wdin orbital self-interaction correction to magnetic exchange couplings. Journal of Chemical Physics, 2018, 149, 164101.	1.2	33
40	NaturalJcoupling (NJC) analysis of the electron lone pair effect on NMR couplings: 2. The anomeric effects on1J(C, H) couplings and its dependence on solvent. Molecular Physics, 2002, 100, 705-715.	0.8	32
41	Anomeric Effect on Geminal and VicinalJHHNMR Coupling Constants. Journal of Physical Chemistry A, 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. Journal of Chemical Physics, 2013, 138, 174115.	1.2	31
43	Shrinking Self-Interaction Errors with the Fermiâ€“LÃ¶wdin Orbital Self-Interaction-Corrected Density Functional Approximation. Journal of Physical Chemistry A, 2018, 122, 9307-9315.	1.1	30
44	The effect of self-interaction error on electrostatic dipoles calculated using density functional theory. Journal of Chemical Physics, 2019, 151, 174106.	1.2	29
45	Scalar relativistic all-electron density functional calculations on periodic systems. Journal of Chemical Physics, 2005, 122, 084108.	1.2	28
46	Magnetization Dynamics from Time-Dependent Noncollinear Spin Density Functional Theory Calculations. Journal of Chemical Theory and Computation, 2015, 11, 3661-3668.	2.3	28
47	DFT-GIAO and DFT-NBO studies of the origin of19F NMR shielding effects in alkyl fluorides. Magnetic Resonance in Chemistry, 1999, 37, 167-172.	1.1	27
48	Self-interaction-free electric dipole polarizabilities for atoms and their ions using the Fermi-LÃ¶wdin self-interaction correction. Physical Review A, 2019, 100, .	1.0	27
49	Finite perturbation theory-density functional theory calculation of the spin-dipolar contribution to NMR spin-spin coupling constants. Molecular Physics, 2001, 99, 655-661.	0.8	26
50	Density Functional Theory Calculation of Indirect Nuclear Magnetic Resonance Spinâˆ’Spin Coupling Constants in C70. Journal of the American Chemical Society, 2004, 126, 7428-7429.	6.6	26
51	Vicinal NMR Protonâˆ’Proton Coupling Constants. An NBO Analysis. Journal of Physical Chemistry A, 2001, 105, 5298-5303.	1.1	25
52	On the Capriciousness of the FCCF Karplus Curve. Journal of the American Chemical Society, 2002, 124, 9702-9703.	6.6	25
53	Magnetic exchange couplings from noncollinear spin density functional perturbation theory. Journal of Chemical Physics, 2008, 129, 194107.	1.2	24
54	A step in the direction of resolving the paradox of Perdewâ€“Zunger self-interaction correction. II. Gauge consistency of the energy density at three levels of approximation. Journal of Chemical Physics, 2020, 152, 214109.	1.2	23

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55	On the Question of the Total Energy in the Fermiâ€“LÃ¶wdin Orbital Self-Interaction Correction Method. Journal of Chemical Theory and Computation, 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. Computational and Theoretical Chemistry, 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. International Journal of Molecular Sciences, 2003, 4, 93-106.	1.8	21
58	Interpretation and Automatic Generation of Fermiâ€Orbital Descriptors. Journal of Computational Chemistry, 2019, 40, 2843-2857.	1.5	21
59	A DFT/GIAO/NBO and experimental study of13C SCSs in 1-X-bicyclo[1.1.1]pentanes. Magnetic Resonance in Chemistry, 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. Journal of Computational Chemistry, 2001, 22, 1615-1621.	1.5	20
61	Theoretical study of charge transfer interactions in methanol adsorbed on magnesium oxide. Surface Science, 2002, 504, 235-243.	0.8	19
62	Computation and analysis of19F substituent chemical shifts of some bridgehead-substituted polycyclic alkyl fluorides. Magnetic Resonance in Chemistry, 2003, 41, 503-508.	1.1	18
63	Magnetic exchange couplings from constrained density functional theory: An efficient approach utilizing analytic derivatives. Journal of Chemical Physics, 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. Polyhedron, 2020, 176, 114194.	1.0	18
65	Prediction of vicinal protonâ€“proton coupling constants³J_{HH}from density functional theory calculations. Molecular Physics, 2005, 103, 1307-1326.	0.8	16
66	Analytic atomic gradients in the fermiâ€Ã¶wdin orbital selfâ€interaction correction. Journal of Computational Chemistry, 2019, 40, 820-825.	1.5	16
67	Magnetic exchange couplings evaluated with Rung 3.5 density functionals. Journal of Chemical Physics, 2011, 134, 214101.	1.2	14
68	Magnetic Couplings in Spin Frustrated Fe7III Disklike Clusters. Journal of Chemical Theory and Computation, 2013, 9, 5585-5589.	2.3	14
69	Magnetic Properties of Mononuclear Co(II) Complexes with Carborane Ligands. Inorganic Chemistry, 2018, 57, 7763-7769.	1.9	14
70	How well do self-interaction corrections repair the overestimation of static polarizabilities in density functional calculations?. Physical Chemistry Chemical Physics, 2021, 23, 18678-18685.	1.3	14
71	Structural dependence of magnetic exchange coupling parameters in transition-metal complexes. Chemical Physics Letters, 2013, 557, 110-113.	1.2	13
72	Magnetic Exchange Couplings in Heterodinuclear Complexes Based on Differential Local Spin Rotations. Journal of Chemical Theory and Computation, 2016, 12, 1728-1734.	2.3	13

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73	On the convergence of FPT-DFT calculations of the Fermi contact contribution to NMR coupling constants. Theoretical Chemistry Accounts, 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. Magnetic Resonance in Chemistry, 1999, 37, 227-231.	1.1	11
75	Graphene Nanoribbons-Based Ultrasensitive Chemical Detectors. Journal of Physical Chemistry C, 2016, 120, 3791-3797.	1.5	11
76	Magnetic Properties of Co(II) Complexes with Polyhedral Carborane Ligands. Inorganic Chemistry, 2019, 58, 2550-2557.	1.9	11
77	Magnetic Exchange Couplings from Noncollinear Perturbation Theory: Dinuclear Cu^{II} Complexes. Journal of Physical Chemistry A, 2014, 118, 5841-5847.	1.1	10
78	Iron(III)â€“Oxo Cluster Chemistry with Dimethylarsinate Ligands: Structures, Magnetic Properties, and Computational Studies. Inorganic Chemistry, 2020, 59, 18090-18101.	1.9	10
79	Density-related properties from self-interaction corrected density functional theory calculations. Journal of Chemical Physics, 2021, 154, 024102.	1.2	8
80	Gradient copolymers of thiophene and pyrrole for photovoltaics. Computational Materials Science, 2015, 96, 69-71.	1.4	7
81	Local Noncollinear Spin Analysis. Journal of Chemical Theory and Computation, 2017, 13, 6101-6107.	2.3	7
82	Atomic structure and Mott nature of the insulating charge density wave phase of 1T-TaS₂. Journal of Physics Condensed Matter, 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. Journal of Physical Chemistry A, 2022, 126, 1923-1935.	1.1	6
84	Substituent effects on scalarJ(13C,13C) couplings in pyrimidines. An experimental and DFT study. Magnetic Resonance in Chemistry, 2004, 42, 938-943.	1.1	5
85	Molecular spin frustration in mixed-chelate Fe5 and Fe6 oxo clusters with high ground state spin values. Polyhedron, 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. Inorganic Chemistry, 0, , .	1.9	5
87	A simple spectrophotometric method to determine phytic acid in poultry wastewater without acid digestion. International Journal of Environmental Analytical Chemistry, 2020, , 1-11.	1.8	4
88	Initial Fermi orbital descriptors for FLOSIC calculations: The quick-FOD method. Chemical Physics Letters, 2021, 780, 138952.	1.2	4
89	Magnetic control over the fundamental structure of atomic wires. Nature Communications, 2022, 13, .	5.8	4
90	Electrostatic effect of the polar bond-polarizable bond interaction on13C chemical shifts. International Journal of Quantum Chemistry, 1998, 70, 105-112.	1.0	3

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91	The polar bondâ€“polarizable bond interaction in 1-X,2-methoxy naphthalenes. An experimental and theoretical study. Journal of Molecular Structure, 2000, 556, 263-273.	1.8	3
92	Theoretical NMR nJ(13C,13C) Scalar Couplings as Probes to Study Diamagnetic Ring Currents in Fullerenes. Advances in Quantum Chemistry, 2005, , 127-139.	0.4	3
93	The performance of density functional approximations for the structures and relative energies of minimum energy crossing points. Chemical Physics Letters, 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. Polyhedron, 2020, 176, 114257.	1.0	2
96	Fermiâ€“LÃ¶wdin orbital self-interaction correction of adsorption energies on transition metal ions. Journal of Chemical Physics, 2022, 156, 134102.	1.2	2
97	Comment on â€œAdditional Insights Between Fermi-LÃ¶wdin Orbital SIC and the Localization Equation Constraints in SIC-DFTâ€. Journal of Physical Chemistry A, 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. Polyhedron, 2022, 225, 116045.	1.0	1
99	Advances in Theoretical and Physical Aspects of Spinâ€”Spin Coupling Constants. ChemInform, 2005, 36, no.	0.1	0
100	Site-specific polarizabilities from analytic linear-response theory. Chemical Physics Letters, 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