Pedro Salvador Sedano

List of Publications by Year
in descending order

79 papers	3,006 citations	172386 29 h-index	175177 52 g-index
80 all docs	80 docs citations	80 times ranked	2687 citing authors

#	Article	IF	Citations
1	Overlap populations, bond orders and valences for â€˜fuzzyâ€™ atoms. Chemical Physics Letters, 2004, 383, 368-375.	1.2	319
2	Electron sharing indexes at the correlated level. Application to aromaticity calculations. Faraday Discussions, 2007, 135, 325-345.	1.6	203
3	Comparison of the AIM Delocalization Index and the Mayer and Fuzzy Atom Bond Orders. Journal of Physical Chemistry A, 2005, 109, 9904-9910.	1.1	169
4	Polarizability of the nitrate anion and its solvation at the air/water interface. Physical Chemistry Chemical Physics, 2003, 5, 3752.	1.3	129
5	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	1.5	113
6	On the effect of the BSSE on intermolecular potential energy surfaces. Comparison ofa priori anda posteriori BSSE correction schemes. Journal of Computational Chemistry, 2001, 22, 765-786.	1.5	93
7	Separation of dynamic and nondynamic correlation. Physical Chemistry Chemical Physics, 2016, 18, 24015-24023.	1.3	85
8	One- and two-center energy components in the atoms in molecules theory. Journal of Chemical Physics, 2001, 115, 1153-1157.	1.2	80
9	Oxidation States from Wave Function Analysis. Journal of Chemical Theory and Computation, 2015, 11, 1501-1508.	2.3	78
10	Energy partitioning for â€œfuzzyâ€•atoms. Journal of Chemical Physics, 2004, 120, 5046-5052.	1.2	77
11	Aromaticity Measures from Fuzzy-Atom Bond Orders (FBO). The Aromatic Fluctuation (FLU) and the para-Delocalization (PDI) Indexes. Journal of Physical Chemistry A, 2006, 110, 5108-5113.	1.1	76
12	Intramolecular basis set superposition error effects on the planarity of benzene and other aromatic molecules: A solution to the problem. Journal of Chemical Physics, 2008, 128, 144108.	1.2	72
13	The Molecular Basis for Antimicrobial Activity of Pore-Forming CyclicÂPeptides. Biophysical Journal, 2011, 100, 2422-2431.	0.2	72
14	Basis set superposition error-counterpoise corrected potential energy surfaces. Application to hydrogen peroxideâ‹¯X (X=Fâ‹¯,â€ŠClâ‹¯, Brâ‹¯,â€ŠLi+,â€ŠNa+) complexes. Journal of Chemical Physics, 1999, 110, 11806-11813.	1.2	71
15	Câ€“Hâ‹¯O H-bonded complexes: How does basis set superposition error change their potential-energy surfaces?. Journal of Chemical Physics, 2000, 113, 5666-5674.	1.2	51
16	Toward a Unique Definition of the Local Spin. Journal of Chemical Theory and Computation, 2012, 8, 1270-1279.	2.3	51
17	Intermolecular bond lengths: extrapolation to the basis set limit on uncorrected and BSSE-corrected potential energy hypersurfaces. Journal of Computational Chemistry, 2001, 22, 196-207.	1.5	49
18	Counterpoise-corrected geometries and harmonic frequencies ofN-body clusters: Application to (HF)nâ€Š(n=3,4). Journal of Chemical Physics, 2003, 118, 537-549.	1.2	48

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19	On the quality of the hardness kernel and the Fukui function to evaluate the global hardness. Journal of Computational Chemistry, 2007, 28, 574-583.	1.5	48
20	Calculation of trans-Hydrogen-Bond13Câ˜'15N Three-Bond and Other ScalarJ-Couplings in Cooperative Peptide Models. A Density Functional Theory Study. Journal of the American Chemical Society, 2004, 126, 14190-14197.	6.6	47
21	Counterpoise Corrected Ion/Molecule Complexes Using Two or Three Fragments. Journal of Physical Chemistry A, 2002, 106, 6883-6889.	1.1	46
22	Communication: An approximation to Bader's topological atom. Journal of Chemical Physics, 2013, 139, 071103.	1.2	46
23	An Objective Alternative to IUPAC's Approach To Assign Oxidation States. Angewandte Chemie - International Edition, 2018, 57, 10525-10529.	7.2	43
24	Density functional energy decomposition into one- and two-atom contributions. Journal of Chemical Physics, 2005, 122, 244110.	1.2	36
25	Performance of 3Dâ€spaceâ€based atomsâ€inâ€molecules methods for electronic delocalization aromaticity indices. Journal of Computational Chemistry, 2011, 32, 386-395.	1.5	36
26	Analysis of the Relative Stabilities of Ortho, Meta, and Para MClÝ(XC₄H₄)(PH₃)₂ Heterometallabenzenes (M = Rh,) Tj ETQq1 0 0 rgBT/Overloc	1.1	36
27	The hardness kernel as the basis for global and local reactivity indices. Journal of Computational Chemistry, 2008, 29, 1064-1072.	1.5	34
28	Not Guilty on Every Count: The â€œNonâ€Innocentâ€•Nitrosyl Ligand in the Framework of IUPACâ€²s Oxidationâ€State Formalism. Angewandte Chemie - International Edition, 2020, 59, 12381-12386.	7.2	33
29	Local spins: improved Hilbert-space analysis. Physical Chemistry Chemical Physics, 2012, 14, 15291.	1.3	30
30	Local Spin Analysis and Chemical Bonding. Chemistry - A European Journal, 2013, 19, 15267-15275.	1.7	29
31	A new tuned range-separated density functional for the accurate calculation of second hyperpolarizabilities. Physical Chemistry Chemical Physics, 2020, 22, 11871-11880.	1.3	28
32	Scrutinizing the Noninnocence of Quinone Ligands in Ruthenium Complexes: Insights from Structural, Electronic, Energy, and Effective Oxidation State Analyses. Inorganic Chemistry, 2016, 55, 2185-2199.	1.9	27
33	Facing the Challenges of Borderline Oxidation State Assignments Using State-of-the-Art Computational Methods. Inorganic Chemistry, 2020, 59, 15410-15420.	1.9	27
34	Direct Calculation oftrans-Hydrogen-Bond13C-15N 3-Bond J-Couplings in Entire Polyalanine Î±-Helices. A Density Functional Theory Study. Journal of Physical Chemistry B, 2007, 111, 2398-2403.	1.2	26
35	The effect of counterpoise correction and relaxation energy term to the internal rotation barriers: Application to the BF3â‹¯NH3 and C2H4â‹¯SO2 dimers. Journal of Chemical Physics, 1999, 111, 4460-4465.	1.2	25
36	The atomic orbitals of the topological atom. Journal of Chemical Physics, 2013, 138, 214107.	1.2	25

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37	The oxidation state in low-valent beryllium and magnesium compounds. Chemical Science, 2022, 13, 6583-6591.	3.7	25
38	Effect of basis set superposition error on the electron density of molecular complexes. Journal of Chemical Physics, 2000, 112, 10106-10115.	1.2	24
39	Insights into mechanism and selectivity in ruthenium(<scp>ii</scp>)-catalysed ortho-arylation reactions directed by Lewis basic groups. Catalysis Science and Technology, 2018, 8, 3174-3182.	2.1	24
40	The Effect of Aqueous Solvation upon Î±-Helix Formation for Polyalanines. Journal of Physical Chemistry B, 2007, 111, 7462-7466.	1.2	23
41	Intramolecular Basis Set Superposition Error Effects on the Planarity of DNA and RNA Nucleobases. Journal of Chemical Theory and Computation, 2009, 5, 2574-2581.	2.3	23
42	An Objective Alternative to IUPAC's Approach To Assign Oxidation States. Angewandte Chemie, 2018, 130, 10685-10689.	1.6	23
43	Beyond the Classical Electronâ€Sharing and Dative Bond Picture: Case of the Spinâ€Polarized Bond. Angewandte Chemie - International Edition, 2021, 60, 1498-1502.	7.2	23
44	One- and two-center physical space partitioning of the energy in the density functional theory. Journal of Chemical Physics, 2007, 126, 234113.	1.2	19
45	Density functional study of ternary Fe x Co y Ni z (xÂ+ÂyÂ+ÂzÂ=Â7) clusters. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	19
46	Computational Monitoring of Oxidation States in Olefin Metathesis. Organometallics, 2019, 38, 4585-4592.	1.1	19
47	Ab initio energy partitioning at the correlated level. Chemical Physics Letters, 2006, 430, 204-209.	1.2	18
48	Effective atomic orbitals for fuzzy atoms. Journal of Chemical Physics, 2009, 130, 234106.	1.2	17
49	Two new constraints for the cumulant matrix. Journal of Chemical Physics, 2014, 141, 234101.	1.2	17
50	Diradical character from the local spin analysis. Physical Chemistry Chemical Physics, 2014, 16, 9565.	1.3	17
51	Rational Design of Cyclic Antimicrobial Peptides Based on BPC194 and BPC198. Molecules, 2017, 22, 1054.	1.7	16
52	Oxidation State Localized Orbitals: A Method for Assigning Oxidation States Using Optimally Fragment-Localized Orbitals and a Fragment Orbital Localization Index. Journal of Chemical Theory and Computation, 2022, 18, 309-322.	2.3	16
53	Second-order MÃ¸llerâ€“Plesset perturbation theory without basis set superposition error. â€ŠII. Open-shell systems. Journal of Chemical Physics, 2004, 120, 5882-5889.	1.2	14
54	Dependence upon Basis Sets of trans Hydrogen-Bond 13Câ‹¯15N 3-Bond and Other Scalar J-Couplings in Amide Dimers Used as Peptide Models. A Density Functional Theory Study. Journal of Physical Chemistry B, 2004, 108, 15370-15375.	1.2	14

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55	Dependencies of J-Couplings upon Dihedral Angles on Proteins. Annual Reports on NMR Spectroscopy, 2014, 81, 185-227.	0.7	14
56	Can We Safely Obtain Formal Oxidation States from Centroids of Localized Orbitals?. Molecules, 2020, 25, 234.	1.7	14
57	KnÃ¶ker Iron Catalysts for Hydrogenation Revisited: A Nonspectator Solvent and Fine-Tuning. Organometallics, 2022, 41, 1204-1215.	1.1	14
58	Bonding description of the Harpoon mechanism. Molecular Physics, 2016, 114, 1345-1355.	0.8	13
59	Bent and Linear {CoNO}⁸ Entities: Structure and Bonding in a Prototypic Class of Nitrosyls. Inorganic Chemistry, 2021, 60, 15980-15996.	1.9	12
60	Dissecting the Hindered Rotation of Ethane. ChemPhysChem, 2009, 10, 1987-1992.	1.0	10
61	Bonding Quandary in the [Cu₃S₂]³⁺ Core: Insights from the Analysis of Domain Averaged Fermi Holes and the Local Spin. Journal of Physical Chemistry A, 2013, 117, 1975-1982.	1.1	10
62	A Fuzzy-Atom Analysis of Electron Delocalization on Hydrogen Bonds. Journal of Physical Chemistry A, 2014, 118, 1142-1149.	1.1	10
63	Nicht in jedem Punkt schuldig: Der â€œnichtâ€•unschuldigeâ€•Nitrosylâ€•Ligand in IUPACs Oxidationsstufenâ€•Empfehlung. Angewandte Chemie, 2020, 132, 12480-12485.	1.6	10
64	Excess charge delocalization in organic and biological molecules: some theoretical notions. Theoretical Chemistry Accounts, 2009, 123, 29-40.	0.5	9
65	J-coupling constants for a trialanine peptide as a function of dihedral angles calculated by density functional theory over the full Ramachandran space. Physical Chemistry Chemical Physics, 2011, 13, 17484.	1.3	9
66	Benchmark calculations of metal carbonyl cations: relativistic vs. electron correlation effects. Physical Chemistry Chemical Physics, 2013, 15, 20080.	1.3	9
67	Characterization and Quantification of Polyradical Character. Journal of Chemical Theory and Computation, 2014, 10, 634-641.	2.3	9
68	Unveiling the Electronic Structure of the Bi(+1)/Bi(+3) Redox Couple on NCN and NNN Pincer Complexes. Inorganic Chemistry, 2021, 60, 17657-17668.	1.9	9
69	A chemical Hamiltonian approach study of the basis set superposition error changes on electron densities and one- and two-center energy components. Journal of Chemical Physics, 2002, 116, 6443-6457.	1.2	8
70	A general efficient implementation of the BSSE-free SCF and MP2 methods based on the chemical Hamiltonian approach. Journal of Computational Chemistry, 2006, 27, 1505-1516.	1.5	8
71	Structural dependencies of protein backbone ²J_{NCâ€²} couplings. Protein Science, 2008, 17, 768-776.	3.1	7
72	Ãœber die klassische Elektronenpaarâ€•und die dative Bindung hinaus: Die Spinâ€•polarisierte Bindung. Angewandte Chemie, 2021, 133, 1520-1524.	1.6	6

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73	Origin-Independent Decomposition of the Static Polarizability. Journal of Chemical Theory and Computation, 2021, 17, 1098-1105.	2.3	6
74	BSSE-free hardness profiles of hydrogen bond exchange in the hydrogen fluoride dimer. International Journal of Quantum Chemistry, 2006, 106, 2910-2919.	1.0	4
75	Accurate ⁵⁷Fe MÃ¶ssbauer Parameters from General Gaussian Basis Sets. Journal of Chemical Theory and Computation, 2021, 17, 7724-7731.	2.3	3
76	Convergence acceleration techniques for nonâ€Hermitian SCF problems. International Journal of Quantum Chemistry, 2009, 109, 2564-2571.	1.0	1
77	A basis set superposition errorâ€free secondâ€order perturbation theory from Hermitian chemical Hamiltonian approach <scp>selfâ€consistent field</scp> canonic orbitals. International Journal of Quantum Chemistry, 2022, 122, e26777.	1.0	1
78	Cageâ€size effects on the encapsulation of <scp> P ₂ </scp> by fullerenes. Journal of Computational Chemistry, 2022, , .	1.5	1
79	Quantitative assessment of the effect of basis set superposition error on the electron density of molecular complexes by means of quantum molecular similarity measures. International Journal of Quantum Chemistry, 2009, 109, 2572-2580.	1.0	0