Pedro Salvador Sedano

List of Publications by Citations

74 papers	2,344 citations	27 h-index	46 g-index
80 ext. papers	2,709 ext. citations	4.4 avg, IF	5.1 L-index

#	Paper	IF	Citations
74	Overlap populations, bond orders and valences for fuzzy atoms. *Chemical Physics Letters*, **2004**, 383, 368-375	2.5	235
73	Electron sharing indexes at the correlated level. Application to aromaticity calculations. *Faraday Discussions*, **2007**, 135, 325-45; discussion 367-401, 503-6	3.6	178
72	Polarizability of the nitrate anion and its solvation at the air/water interface. *Physical Chemistry Chemical Physics*, **2003**, 5, 3752	3.6	119
71	Comparison of the AIM delocalization index and the Mayer and fuzzy atom bond orders. *Journal of Physical Chemistry A*, **2005**, 109, 9904-10	2.8	117
70	On the effect of the BSSE on intermolecular potential energy surfaces. Comparison of a priori and a posteriori BSSE correction schemes. *Journal of Computational Chemistry*, **2001**, 22, 765-786	3.5	89
69	One- and two-center energy components in the atoms in molecules theory. *Journal of Chemical Physics*, **2001**, 115, 1153-1157	3.9	72
68	Nine questions on energy decomposition analysis. *Journal of Computational Chemistry*, **2019**, 40, 2248-2283	3.5	70
67	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	3.9	70
66	Energy partitioning for "fuzzy" atoms. *Journal of Chemical Physics*, **2004**, 120, 5046-52	3.9	66
65	Basis set superposition error-counterpoise corrected potential energy surfaces. Application to hydrogen peroxide?X (X=F Cl Br Li+, Na+) complexes. *Journal of Chemical Physics*, **1999**, 110, 11806-11813	3.9	61
64	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, 5108-13	2.8	60
63	The molecular basis for antimicrobial activity of pore-forming cyclic peptides. *Biophysical Journal*, **2011**, 100, 2422-31	2.9	58
62	Separation of dynamic and nondynamic correlation. *Physical Chemistry Chemical Physics*, **2016**, 18, 24015-23	3.3	53
61	CH?O H-bonded complexes: How does basis set superposition error change their potential-energy surfaces?. *Journal of Chemical Physics*, **2000**, 113, 5666-5674	3.9	50
60	Oxidation States from Wave Function Analysis. *Journal of Chemical Theory and Computation*, **2015**, 11, 1501-8	6.4	46
59	Counterpoise-corrected geometries and harmonic frequencies of N-body clusters: Application to (HF)n (n=3,4). *Journal of Chemical Physics*, **2003**, 118, 537-549	3.9	46
58	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	3.5	46

57	Counterpoise Corrected Ion/Molecule Complexes Using Two or Three Fragments. *Journal of Physical Chemistry A*, **2002**, 106, 6883-6889	2.8	46
56	Toward a Unique Definition of the Local Spin. *Journal of Chemical Theory and Computation*, **2012**, 8, 12769	5.4	45
55	Calculation of trans-hydrogen-bond 13C-15N three-bond and other scalar J-couplings in cooperative peptide models. A density functional theory study. *Journal of the American Chemical Society*, **2004**, 126, 14190-7	16.4	45
54	On the quality of the hardness kernel and the Fukui function to evaluate the global hardness. *Journal of Computational Chemistry*, **2007**, 28, 574-83	3.5	44
53	Communication: An approximation to Bader's topological atom. *Journal of Chemical Physics*, **2013**, 139, 071103	3.9	34
52	Density functional energy decomposition into one- and two-atom contributions. *Journal of Chemical Physics*, **2005**, 122, 244110	3.9	34
51	Performance of 3D-space-based atoms-in-molecules methods for electronic delocalization aromaticity indices. *Journal of Computational Chemistry*, **2011**, 32, 386-95	3.5	33
50	Local spin analysis and chemical bonding. *Chemistry - A European Journal*, **2013**, 19, 15267-75	4.8	27
49	Local spins: improved Hilbert-space analysis. *Physical Chemistry Chemical Physics*, **2012**, 14, 15291-8	3.6	27
48	The hardness kernel as the basis for global and local reactivity indices. *Journal of Computational Chemistry*, **2008**, 29, 1064-72	3.5	27
47	Analysis of the Relative Stabilities of Ortho, Meta, and Para MClY(XC4H4)(PH3)2Heterometallabenzenes (M = Rh, Ir; X = N, P; Y = Cl and M = Ru, Os; X = N, P; Y = CO). *Organometallics*, **2013**, 32, 4892-4903	3.8	26
46	The effect of counterpoise correction and relaxation energy term to the internal rotation barriers: Application to the BF3?NH3 and C2H4?SO2 dimers. *Journal of Chemical Physics*, **1999**, 111, 4460-4465	3.9	24
45	An Objective Alternative to IUPAC's Approach To Assign Oxidation States. *Angewandte Chemie - International Edition*, **2018**, 57, 10525-10529	16.4	24
44	Effect of basis set superposition error on the electron density of molecular complexes. *Journal of Chemical Physics*, **2000**, 112, 10106-10115	3.9	23
43	The effect of aqueous solvation upon alpha-helix formation for polyalanines. *Journal of Physical Chemistry B*, **2007**, 111, 7462-6	3.4	22
42	Intramolecular Basis Set Superposition Error Effects on the Planarity of DNA and RNA Nucleobases. *Journal of Chemical Theory and Computation*, **2009**, 5, 2574-81	6.4	21
41	Scrutinizing the Noninnocence of Quinone Ligands in Ruthenium Complexes: Insights from Structural, Electronic, Energy, and Effective Oxidation State Analyses. *Inorganic Chemistry*, **2016**, 55, 2185-99	5.1	19
40	Insights into mechanism and selectivity in ruthenium(II)-catalysed ortho-arylation reactions directed by Lewis basic groups. *Catalysis Science and Technology*, **2018**, 8, 3174-3182	5.5	18

39	An Objective Alternative to IUPAC's Approach To Assign Oxidation States. *Angewandte Chemie*, **2018**, 130, 10685-10689	3.6	18
38	Density functional study of ternary Fe x Co y Ni z (x + y + z = 7) clusters. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	17
37	Direct calculation of trans-hydrogen-bond 13C-15N 3-bond J-couplings in entire polyalanine alpha-helices. A density functional theory study. *Journal of Physical Chemistry B*, **2007**, 111, 2398-403	3.4	17
36	Ab initio energy partitioning at the correlated level. *Chemical Physics Letters*, **2006**, 430, 204-209	2.5	17
35	Two new constraints for the cumulant matrix. *Journal of Chemical Physics*, **2014**, 141, 234101	3.9	16
34	Not Guilty on Every Count: The "Non-Innocent" Nitrosyl Ligand in the Framework of IUPAC's Oxidation-State Formalism. *Angewandte Chemie - International Edition*, **2020**, 59, 12381-12386	16.4	15
33	Diradical character from the local spin analysis. *Physical Chemistry Chemical Physics*, **2014**, 16, 9565-71	3.6	15
32	Effective atomic orbitals for fuzzy atoms. *Journal of Chemical Physics*, **2009**, 130, 234106	3.9	15
31	One- and two-center physical space partitioning of the energy in the density functional theory. *Journal of Chemical Physics*, **2007**, 126, 234113	3.9	14
30	Dependence upon Basis Sets of trans Hydrogen-Bond 13C□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	3.4	14
29	The atomic orbitals of the topological atom. *Journal of Chemical Physics*, **2013**, 138, 214107	3.9	13
28	Second-order M□ller-Plesset perturbation theory without basis set superposition error. II. Open-shell systems. *Journal of Chemical Physics*, **2004**, 120, 5882-9	3.9	13
27	Computational Monitoring of Oxidation States in Olefin Metathesis. *Organometallics*, **2019**, 38, 4585-4592	3.8	12
26	A new tuned range-separated density functional for the accurate calculation of second hyperpolarizabilities. *Physical Chemistry Chemical Physics*, **2020**, 22, 11871-11880	3.6	11
25	Bonding description of the Harpoon mechanism□This paper is dedicated to Andreas Savin on the occasion of his 65th birthday.View all notes. *Molecular Physics*, **2016**, 114, 1345-1355	1.7	11
24	Beyond the Classical Electron-Sharing and Dative Bond Picture: Case of the Spin-Polarized Bond. *Angewandte Chemie - International Edition*, **2021**, 60, 1498-1502	16.4	11
23	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, 1975-82	2.8	10
22	Rational Design of Cyclic Antimicrobial Peptides Based on BPC194 and BPC198. *Molecules*, **2017**, 22,	4.8	10

21	Dependencies of J-Couplings upon Dihedral Angles on Proteins. *Annual Reports on NMR Spectroscopy*, **2014**, 81, 185-227	1.7	9
20	Benchmark calculations of metal carbonyl cations: relativistic vs. electron correlation effects. *Physical Chemistry Chemical Physics*, **2013**, 15, 20080-90	3.6	9
19	Dissecting the hindered rotation of ethane. *ChemPhysChem*, **2009**, 10, 1987-92	3.2	9
18	Can We Safely Obtain Formal Oxidation States from Centroids of Localized Orbitals?. *Molecules*, **2020**, 25,	4.8	8
17	A fuzzy-atom analysis of electron delocalization on hydrogen bonds. *Journal of Physical Chemistry A* , **2014**, 118, 1142-9	2.8	8
16	Characterization and Quantification of Polyradical Character. *Journal of Chemical Theory and Computation*, **2014**, 10, 634-41	6.4	8
15	Excess charge delocalization in organic and biological molecules: some theoretical notions. *Theoretical Chemistry Accounts*, **2009**, 123, 29-40	1.9	8
14	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	3.9	8
13	Facing the Challenges of Borderline Oxidation State Assignments Using State-of-the-Art Computational Methods. *Inorganic Chemistry*, **2020**, 59, 15410-15420	5.1	8
12	Structural dependencies of protein backbone 2JNC' couplings. *Protein Science*, **2008**, 17, 768-76	6.3	7
11	Nicht in jedem Punkt schuldig: Der Nicht-unschuldige Nitrosyl-Ligand in IUPACs Oxidationsstufen-Empfehlung. *Angewandte Chemie*, **2020**, 132, 12480-12485	3.6	7
10	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, 17484-93	3.6	6
9	A general efficient implementation of the BSSE-free SCF and MP2 methods based on the chemical Hamiltonian approach. *Journal of Computational Chemistry*, **2006**, 27, 1505-16	3.5	6
8	BSSE-free hardness profiles of hydrogen bond exchange in the hydrogen fluoride dimer. *International Journal of Quantum Chemistry*, **2006**, 106, 2910-2919	2.1	4
7	Über die klassische Elektronenpaar- und die dative Bindung hinaus: Die Spin-polarisierte Bindung. *Angewandte Chemie*, **2021**, 133, 1520-1524	3.6	3
6	Unveiling the Electronic Structure of the Bi(+1)/Bi(+3) Redox Couple on NCN and NNN Pincer Complexes. *Inorganic Chemistry*, **2021**, 60, 17657-17668	5.1	2
5	Origin-Independent Decomposition of the Static Polarizability. *Journal of Chemical Theory and Computation*, **2021**, 17, 1098-1105	6.4	2
4	Bent and Linear {CoNO} Entities: Structure and Bonding in a Prototypic Class of Nitrosyls. *Inorganic Chemistry*, **2021**, 60, 15980-15996	5.1	0

3	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	2.1
2	Convergence acceleration techniques for non-Hermitian SCF problems. *International Journal of Quantum Chemistry*, **2009**, 109, 2564-2571	2.1
1	A basis set superposition error-free second-order perturbation theory from Hermitian chemical Hamiltonian approach self-consistent field canonic orbitals. *International Journal of Quantum Chemistry*,e26777	2.1