Rafael Lopez Fernandez

List of Publications by Year
in descending order

72	1,122	331670 21	454955 30
papers	citations	h-index	g-index

72	72	72	672
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Reference program for molecular calculations with Slater-type orbitals. Journal of Computational Chemistry, 1998, 19, 1284-1293.	3.3	99
2	Polarized basis sets of Slater-type orbitals: H to Ne atoms. Journal of Computational Chemistry, 2003, 24, 859-868.	3.3	62
3	Efficiency of the algorithms for the calculation of Slater molecular integrals in polyatomic molecules. Journal of Computational Chemistry, 2004, 25, 1987-1994.	3.3	54
4	DAMQT 2.1.0: A new version of the DAMQT package enabled with the topographical analysis of electron density and electrostatic potential in molecules. Journal of Computational Chemistry, 2015, 36, 2350-2359.	3.3	47
5	Analysis of the molecular density. Journal of Chemical Physics, 1999, 110, 4213-4220.	3.0	43
6	Calculation of many-centre two-electron molecular integrals with STO. Computer Physics Communications, 1997, 105, 216-224.	7.5	38
7	Analytical method for the representation of atoms-in-molecules densities. Journal of Computational Chemistry, 2004, 25, 1355-1363.	3.3	36
8	Improvements in DFT Calculations of Spinâ€“Spin Coupling Constants. Journal of Chemical Theory and Computation, 2014, 10, 4938-4949.	5.3	31
9	Electron density analysis of 1-butyl-3-methylimidazolium chloride ionic liquid. Journal of Molecular Modeling, 2014, 20, 2175.	1.8	31
10	Analysis of the molecular density: STO densities. Journal of Chemical Physics, 2002, 117, 533-540.	3.0	29
11	Restricted Hartree-Fock approximation. I. Techniques for the energy minimization. Journal of Computational Chemistry, 1983, 4, 33-40.	3.3	26
12	Chemical Notions from the Electron Density. Journal of Chemical Theory and Computation, 2005, 1, 1083-1095.	5.3	26
13	Density Functional Theory Study of Ionic Liquid Adsorption on Circumcoronene Shaped Graphene. Journal of Physical Chemistry C, 2018, 122, 2624-2631.	3.1	26
14	An improved program for molecular calculations with B functions. Computational and Theoretical Chemistry, 1999, 490, 201-217.	1.5	25
15	Topology of molecular electron density and electrostatic potential with DAMQT. Computer Physics Communications, 2017, 214, 207-215.	7.5	25
16	Accurate gaussian expansion of STO's. Test of many-center slater integrals. Collection of Czechoslovak Chemical Communications, 1988, 53, 2250-2265.	1.0	23
17	Improved algorithm for the calculation of one-electron two-center integrals with STOs. Journal of Computational Chemistry, 1989, 10, 869-874.	3.3	23
18	Electrostatic potentials and fields from density expansions of deformed atoms in molecules. Journal of Computational Chemistry, 2004, 25, 1347-1354.	3.3	23

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19	DAMQT: A package for the analysis of electron density in molecules. Computer Physics Communications, 2009, 180, 1654-1660.	7.5	23
20	Statistical Refinement and Fitting of Experimental Viscosity-to-Temperature Data in Ionic Liquids. Industrial & Engineering Chemistry Research, 2014, 53, 10475-10484.	3.7	23
21	Rotation of real spherical harmonics. Computer Physics Communications, 1989, 52, 323-331.	7.5	21
22	Rapid topography mapping of scalar fields: Large molecular clusters. Journal of Chemical Physics, 2012, 137, 074116.	3.0	21
23	Calculation of two-center one-electron molecular integrals with STOs. Computer Physics Communications, 1991, 64, 329-342.	7.5	19
24	Understanding the Structure and Properties of Cholinium Amino Acid Based Ionic Liquids. Journal of Physical Chemistry B, 2016, 120, 10327-10335.	2.6	19
25	Multiple one-center expansions of charge distributions associated with Slater orbitals. Computational and Theoretical Chemistry, 1998, 433, 7-18.	1.5	18
26	The role of errors related to DFT methods in calculations involving ion pairs of ionic liquids. Journal of Computational Chemistry, 2017, 38, 530-540.	3.3	18
27	Translation of STO charge distributions. Journal of Computational Chemistry, 2005, 26, 846-855.	3.3	16
28	Effect of the molecular structure in the prediction of thermodynamic properties for 1â€butylâ€3â€methylimidazolium chloride ionic liquid. International Journal of Quantum Chemistry, 2013, 113, 852-858.	2.0	16
29	DAMQT 2.0: A new version of the DAMQT package for the analysis of electron density in molecules. Computer Physics Communications, 2015, 192, 289-294.	7.5	15
30	Deformed atoms in molecules: analytical representation of atomic densities for Gaussian type orbitals. Computational and Theoretical Chemistry, 2005, 727, 115-121.	1.5	14
31	Auxiliary functions for molecular integrals with Slater-type orbitals. I. Translation methods. International Journal of Quantum Chemistry, 2006, 106, 1986-1997.	2.0	14
32	A mathematical model applied for assisting the estimation of PMI in a case of forensic importance. First record of Conicera similis (Diptera: Phoridae) in a corpse. Forensic Science International, 2013, 231, e11-e18.	2.2	11
33	Towards quantifying the role of exact exchange in the prediction hydrogen bond spin-spin coupling constants involving fluorine. Journal of Chemical Physics, 2016, 145, 084301.	3.0	11
34	Density and binding forces: Rotational barrier of ethane. Journal of Chemical Physics, 2003, 119, 12251-12256.	3.0	10
35	Auxiliary functions for molecular integrals with Slaterâ€type orbitals. II. Gauss transform methods. International Journal of Quantum Chemistry, 2008, 108, 25-39.	2.0	10
36	Repulsion integrals involving Slater-type functions and Yukawa potential. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	10

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37	Alkyl substituent effect on density, viscosity and chemical behavior of 1-alkyl-3-methylimidazolium chloride. Journal of Molecular Modeling, 2014, 20, 2392.	1.8	10
38	Modeling EPR parameters of nitrogen containing conjugated radical cations. RSC Advances, 2015, 5, 62551-62562.	3.6	10
39	Chemical forces in terms of the electron density. Theoretical Chemistry Accounts, 2007, 118, 709-721.	1.4	9
40	Communication: Accurate determination of side-chain torsion angle Ï‡1 in proteins: Phenylalanine residues. Journal of Chemical Physics, 2011, 134, 061101.	3.0	9
41	Translation of real solid spherical harmonics. International Journal of Quantum Chemistry, 2013, 113, 1544-1548.	2.0	9
42	Atomic partitioning of long-range two-center potentials. Computational and Theoretical Chemistry, 1985, 120, 163-174.	1.5	8
43	The Ïƒ-donating and Ï€-accepting properties ofortho-Si(CH3)3phosphinine macrocycles. Heteroatom Chemistry, 2003, 14, 160-169.	0.7	8
44	Generation of basis sets with high degree of fulfillment of the Hellmann-Feynman theorem. Journal of Computational Chemistry, 2007, 28, 748-758.	3.3	8
45	Efficient evaluation of the Fourier transform over products of Slater-type orbitals on different centers. Journal of Physics A: Mathematical and Theoretical, 2008, 41, 485205.	2.1	8
46	Coulomb integrals for Gaussian, Slater, Bessel and polynomial-type functions. Computational and Theoretical Chemistry, 2001, 537, 27-40.	1.5	7
47	Effect of dielectric constant on estimation of properties of ionic liquids: an analysis of 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide. RSC Advances, 2015, 5, 72709-72715.	3.6	7
48	Molecular modeling and physicochemical properties of 1-alkyl-3-methylimidazolium-FeX 4 and -Fe 2 X 7 (X = Cl and Br) magneticÂionic liquids. Journal of Molecular Liquids, 2018, 256, 175-182.	4.9	7
49	Computational Protocol to Evaluate Side-Chain Vicinal Spinâ€“Spin Coupling Constants and Karplus Equation in Amino Acids: Alanine Dipeptide Model. Journal of Chemical Theory and Computation, 2019, 15, 4252-4263.	5.3	7
50	Single-exponent Slater function expansions for lithium to neon atoms. Journal of Physics B: Atomic, Molecular and Optical Physics, 1996, 29, 5273-5282.	1.5	6
51	Accuracy of the electrostatic theorem for high-quality Slater and Gaussian basis sets. International Journal of Quantum Chemistry, 2004, 100, 221-230.	2.0	6
52	Theoretical DFT karplus equations: Amino acid sideâ€chain torsion angle Ï‡₁. International Journal of Quantum Chemistry, 2013, 113, 656-660.	2.0	5
53	Electron density deformations provide new insights into the spectral shift of rhodopsins. Journal of Computational Chemistry, 2013, 34, 2460-2471.	3.3	5
54	Threeâ€center Coulomb repulsion integrals with Slater functions. International Journal of Quantum Chemistry, 2008, 108, 1415-1421.	2.0	4

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55	Generation of Basis Sets for Accurate Molecular Calculations: Application to Helium Atom and Dimer. Computation, 2022, 10, 65.	2.0	4
56	Atomic partitioning of two-center potentials for slater basis. International Journal of Quantum Chemistry, 1986, 29, 1155-1164.	2.0	3
57	Correspondence between GTO and STO molecular basis sets. Journal of Computational Chemistry, 2001, 22, 1655-1665.	3.3	3
58	Electric field integrals for Slater-type orbitals. International Journal of Quantum Chemistry, 2004, 100, 131-141.	2.0	3
59	Improved partitionâ€“expansion of twoâ€center distributions involving slater functions. Journal of Computational Chemistry, 2013, 34, 1800-1809.	3.3	3
60	Performance of wave function and density functional methods for water hydrogen bond spinâ€“spin coupling constants. Journal of Molecular Modeling, 2017, 23, 134.	1.8	3
61	On the molecular electron structure of three phosphinine-containing macrocycles. Journal of Computational Chemistry, 2007, 28, 958-966.	3.3	2
62	Molecular modeling of porphyrin-based conjugates and subphthalocyanine aggregates. Journal of Porphyrins and Phthalocyanines, 2009, 13, 494-508.	0.8	2
63	Direct calculation of the Coulomb matrix: Slater-type orbitals. Theoretical Chemistry Accounts, 2011, 128, 115-125.	1.4	2
64	Nuclear cusp conditions and their fulfillment in molecular calculations with SLATER basis sets. International Journal of Quantum Chemistry, 2014, 114, 1393-1400.	2.0	2
65	Efficient algorithm for expanding theoretical electron densities in canterakisâ€“zernike functions. Journal of Computational Chemistry, 2018, 39, 2022-2032.	3.3	2
66	DAMQT 3: Advanced suite for the analysis of molecular density and related properties in large systems. Computer Physics Communications, 2022, 279, 108460.	7.5	2
67	Multipole moments from the partitionâ€“expansion method. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	1
68	Efficient Evaluation of Molecular Electrostatic Potential in Large Systems. Computation, 2019, 7, 64.	2.0	1
69	Additivity and transferability of exchange energy. International Journal of Quantum Chemistry, 2010, 110, 1137-1141.	2.0	0
70	A note on atomic density. International Journal of Quantum Chemistry, 2013, 113, 52-55.	2.0	0
71	Molecular fingerprints based on Jacobi expansions of electron densities. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	0
72	Analysis of the Electronic Density as a Support of the Concepts of Empirical Structural Chemistry. Topics in Molecular Organization and Engineering, 1989, , 31-47.	0.1	0