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	Generation of Basis Sets for Accurate Molecular Calculations: Application to Helium Atom and Dimer. Computation, 2022, 10, 65.	2.0	4
2	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
3	Molecular fingerprints based on Jacobi expansions of electron densities. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	0
4	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
5	Efficient Evaluation of Molecular Electrostatic Potential in Large Systems. Computation, 2019, 7, 64.	2.0	1
6	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
7	Density Functional Theory Study of Ionic Liquid Adsorption on Circumcoronene Shaped Graphene. Journal of Physical Chemistry C, 2018, 122, 2624-2631.	3.1	26
8	Efficient algorithm for expanding theoretical electron densities in canterakisâ€“zernike functions. Journal of Computational Chemistry, 2018, 39, 2022-2032.	3.3	2
9	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
10	Topology of molecular electron density and electrostatic potential with DAMQT. Computer Physics Communications, 2017, 214, 207-215.	7.5	25
11	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
12	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
13	Understanding the Structure and Properties of Cholinium Amino Acid Based Ionic Liquids. Journal of Physical Chemistry B, 2016, 120, 10327-10335.	2.6	19
14	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
15	Modeling EPR parameters of nitrogen containing conjugated radical cations. RSC Advances, 2015, 5, 62551-62562.	3.6	10
16	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
17	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
18	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

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19	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
20	Improvements in DFT Calculations of Spinâ€“Spin Coupling Constants. Journal of Chemical Theory and Computation, 2014, 10, 4938-4949.	5.3	31
21	Statistical Refinement and Fitting of Experimental Viscosity-to-Temperature Data in Ionic Liquids. Industrial & Engineering Chemistry Research, 2014, 53, 10475-10484.	3.7	23
22	Electron density analysis of 1-butyl-3-methylimidazolium chloride ionic liquid. Journal of Molecular Modeling, 2014, 20, 2175.	1.8	31
23	Theoretical DFT karplus equations: Amino acid sideâ€chain torsion angle Ï‡₁. International Journal of Quantum Chemistry, 2013, 113, 656-660.	2.0	5
24	A note on atomic density. International Journal of Quantum Chemistry, 2013, 113, 52-55.	2.0	0
25	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
26	Electron density deformations provide new insights into the spectral shift of rhodopsins. Journal of Computational Chemistry, 2013, 34, 2460-2471.	3.3	5
27	Multipole moments from the partitionâ€“expansion method. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	1
28	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
29	Translation of real solid spherical harmonics. International Journal of Quantum Chemistry, 2013, 113, 1544-1548.	2.0	9
30	Repulsion integrals involving Slater-type functions and Yukawa potential. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	10
31	Improved partitionâ€“expansion of twoâ€center distributions involving slater functions. Journal of Computational Chemistry, 2013, 34, 1800-1809.	3.3	3
32	Rapid topography mapping of scalar fields: Large molecular clusters. Journal of Chemical Physics, 2012, 137, 074116.	3.0	21
33	Direct calculation of the Coulomb matrix: Slater-type orbitals. Theoretical Chemistry Accounts, 2011, 128, 115-125.	1.4	2
34	Communication: Accurate determination of side-chain torsion angle Ï‡1 in proteins: Phenylalanine residues. Journal of Chemical Physics, 2011, 134, 061101.	3.0	9
35	Additivity and transferability of exchange energy. International Journal of Quantum Chemistry, 2010, 110, 1137-1141.	2.0	0
36	Molecular modeling of porphyrin-based conjugates and subphthalocyanine aggregates. Journal of Porphyrins and Phthalocyanines, 2009, 13, 494-508.	0.8	2

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37	DAMQT: A package for the analysis of electron density in molecules. Computer Physics Communications, 2009, 180, 1654-1660.	7.5	23
38	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
39	Threeâ€center Coulomb repulsion integrals with Slater functions. International Journal of Quantum Chemistry, 2008, 108, 1415-1421.	2.0	4
40	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
41	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
42	On the molecular electron structure of three phosphinine-containing macrocycles. Journal of Computational Chemistry, 2007, 28, 958-966.	3.3	2
43	Chemical forces in terms of the electron density. Theoretical Chemistry Accounts, 2007, 118, 709-721.	1.4	9
44	Auxiliary functions for molecular integrals with Slater-type orbitals. I. Translation methods. International Journal of Quantum Chemistry, 2006, 106, 1986-1997.	2.0	14
45	Deformed atoms in molecules: analytical representation of atomic densities for Gaussian type orbitals. Computational and Theoretical Chemistry, 2005, 727, 115-121.	1.5	14
46	Translation of STO charge distributions. Journal of Computational Chemistry, 2005, 26, 846-855.	3.3	16
47	Chemical Notions from the Electron Density. Journal of Chemical Theory and Computation, 2005, 1, 1083-1095.	5.3	26
48	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
49	Electric field integrals for Slater-type orbitals. International Journal of Quantum Chemistry, 2004, 100, 131-141.	2.0	3
50	Electrostatic potentials and fields from density expansions of deformed atoms in molecules. Journal of Computational Chemistry, 2004, 25, 1347-1354.	3.3	23
51	Analytical method for the representation of atoms-in-molecules densities. Journal of Computational Chemistry, 2004, 25, 1355-1363.	3.3	36
52	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
53	The Ïƒ-donating and Ï€-accepting properties ofortho-Si(CH3)3phosphinine macrocycles. Heteroatom Chemistry, 2003, 14, 160-169.	0.7	8
54	Polarized basis sets of Slater-type orbitals: H to Ne atoms. Journal of Computational Chemistry, 2003, 24, 859-868.	3.3	62

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55	Density and binding forces: Rotational barrier of ethane. Journal of Chemical Physics, 2003, 119, 12251-12256.	3.0	10
56	Analysis of the molecular density: STO densities. Journal of Chemical Physics, 2002, 117, 533-540.	3.0	29
57	Correspondence between GTO and STO molecular basis sets. Journal of Computational Chemistry, 2001, 22, 1655-1665.	3.3	3
58	Coulomb integrals for Gaussian, Slater, Bessel and polynomial-type functions. Computational and Theoretical Chemistry, 2001, 537, 27-40.	1.5	7
59	An improved program for molecular calculations with B functions. Computational and Theoretical Chemistry, 1999, 490, 201-217.	1.5	25
60	Analysis of the molecular density. Journal of Chemical Physics, 1999, 110, 4213-4220.	3.0	43
61	Multiple one-center expansions of charge distributions associated with Slater orbitals. Computational and Theoretical Chemistry, 1998, 433, 7-18.	1.5	18
62	Reference program for molecular calculations with Slater-type orbitals. Journal of Computational Chemistry, 1998, 19, 1284-1293.	3.3	99
63	Calculation of many-centre two-electron molecular integrals with STO. Computer Physics Communications, 1997, 105, 216-224.	7.5	38
64	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
65	Calculation of two-center one-electron molecular integrals with STOs. Computer Physics Communications, 1991, 64, 329-342.	7.5	19
66	Rotation of real spherical harmonics. Computer Physics Communications, 1989, 52, 323-331.	7.5	21
67	Improved algorithm for the calculation of one-electron two-center integrals with STOs. Journal of Computational Chemistry, 1989, 10, 869-874.	3.3	23
68	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
69	Accurate gaussian expansion of STO's. Test of many-center slater integrals. Collection of Czechoslovak Chemical Communications, 1988, 53, 2250-2265.	1.0	23
70	Atomic partitioning of two-center potentials for slater basis. International Journal of Quantum Chemistry, 1986, 29, 1155-1164.	2.0	3
71	Atomic partitioning of long-range two-center potentials. Computational and Theoretical Chemistry, 1985, 120, 163-174.	1.5	8
72	Restricted Hartree-Fock approximation. I. Techniques for the energy minimization. Journal of Computational Chemistry, 1983, 4, 33-40.	3.3	26