Jose Manuel Garcia De La Vega

List of Publications by Year
in descending order

115 papers	1,629 citations	331670 21 h-index	395702 33 g-index
115 all docs	115 docs citations	115 times ranked	1789 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	Computational approaches to amino acid side-chain conformation using combined NMR theoretical and experimental results: leucine-67 in Desulfovibrio vulgaris flavodoxin. Briefings in Bioinformatics, 2021, 22, .	6.5	2
3	Evolutionary algorithm-based generation of optimum peptide sequences with dengue virus inhibitory activity. Future Medicinal Chemistry, 2021, 13, 993-1000.	2.3	4
4	Toward a Computational NMR Procedure for Modeling Dipeptide Side-Chain Conformation. Journal of Chemical Information and Modeling, 2021, 61, 6012-6023.	5.4	1
5	Role of Augmented Basis Sets and Quest for ab Initio Performance/Cost Alternative to Kohnâ€“Sham Density Functional Theory. Journal of Physical Chemistry A, 2020, 124, 126-134.	2.5	9
6	Accurate atomic momentum integrals and Compton profiles. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 54, 025003.	1.5	0
7	Undersampling: case studies of flaviviral inhibitory activities. Journal of Computer-Aided Molecular Design, 2019, 33, 997-1008.	2.9	6
8	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
9	Density Functional Theory Study of Ionic Liquid Adsorption on Circumcoronene Shaped Graphene. Journal of Physical Chemistry C, 2018, 122, 2624-2631.	3.1	26
10	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
11	Assessing How Correlated Molecular Orbital Calculations Can Perform versus Kohnâ€“Sham DFT: Barrier Heights/Isomerizations. Chemistry - A European Journal, 2017, 23, 9122-9129.	3.3	14
12	Predictions of Physicochemical Properties of Ionic Liquids with DFT. Computation, 2016, 4, 25.	2.0	35
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	Similarity measures between excited singlet and triplet electron densities in linear acenes: an application to singlet fission. Molecular Physics, 2016, 114, 3650-3657.	1.7	1
15	Self-interaction error in DFT-based modelling of ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 2175-2182.	2.8	20
16	Integrating sampling techniques and inverse virtual screening: toward the discovery of artificial peptide-based receptors for ligands. Molecular Diversity, 2016, 20, 421-438.	3.9	7
17	Modeling EPR parameters of nitrogen containing conjugated radical cations. RSC Advances, 2015, 5, 62551-62562.	3.6	10
18	Complexes of nitric oxide with water and imidazole. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	2

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19	Assessment of DFT functionals with fluorineâ€“fluorine coupling constants. Molecular Physics, 2015, 113, 1924-1936.	1.7	15
20	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
21	In silicoAntibacterial Activity Modeling Based on the TOMOCOMD-CARDD Approach. Journal of the Brazilian Chemical Society, 2015, , .	0.6	16
22	Dynamics of the O + ClO Reaction: Reactive and Vibrational Relaxation Processes. Journal of Physical Chemistry A, 2014, 118, 12120-12129.	2.5	1
23	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
24	The absorption spectrum of C60 in n-hexane solution revisited: Fitted experiment and TDDFT/PCM calculations. Chemical Physics Letters, 2014, 593, 72-76.	2.6	14
25	Improvements in DFT Calculations of Spinâ€“Spin Coupling Constants. Journal of Chemical Theory and Computation, 2014, 10, 4938-4949.	5.3	31
26	Single-Sheeted Double Many-Body Expansion Potential Energy Surface for Ground-State ClO₂. Journal of Physical Chemistry A, 2014, 118, 4851-4862.	2.5	6
27	Natural bond orbital/natural J-coupling study of vicinal couplings. Journal of Molecular Modeling, 2014, 20, 2225.	1.8	4
28	Unusual hydrogen bond patterns contributing to supramolecular assembly: conformational study, Hirshfeld surface analysis and density functional calculations of a new steroid derivative. CrystEngComm, 2014, 16, 7802-7814.	2.6	18
29	Electron density analysis of 1-butyl-3-methylimidazolium chloride ionic liquid. Journal of Molecular Modeling, 2014, 20, 2175.	1.8	31
30	Dumbbell-Type Fullerene-Steroid Hybrids: A Join Experimental and Theoretical Investigation for Conformational, Configurational, and Circular Dichroism Assignments. Journal of Organic Chemistry, 2014, 79, 3473-3486.	3.2	13
31	Theoretical DFT karplus equations: Amino acid sideâ€chain torsion angle Ï‡₁. International Journal of Quantum Chemistry, 2013, 113, 656-660.	2.0	5
32	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
33	Analysis of Contributions to Spinâ€“Spin Coupling Constants by the Natural J-Coupling Method. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2013, 3, 161-207.	0.6	4
34	Integration of ligand and structure-based virtual screening for identification of leading anabolic steroids. Journal of Steroid Biochemistry and Molecular Biology, 2013, 138, 348-358.	2.5	3
35	Electron density deformations provide new insights into the spectral shift of rhodopsins. Journal of Computational Chemistry, 2013, 34, 2460-2471.	3.3	5
36	Computational NMR coupling constants: Shifting and scaling factors for evaluating ¹J_{CH}. Magnetic Resonance in Chemistry, 2013, 51, 775-787.	1.9	23

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37	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
38	Extension of the AMBER Force Field for Nitroxide Radicals and Combined QM/MM/PCM Approach to the Accurate Determination of EPR Parameters of DMPO-H in Solution. Journal of Chemical Theory and Computation, 2013, 9, 3626-3636.	5.3	8
39	Theoretical advances on coefficients of relational agreement: application to cheminformatics as kâ€way biomolecular similarity measures. Journal of Chemometrics, 2013, 27, 420-430.	1.3	1
40	Electronic excitations of C60 aggregates. Physical Chemistry Chemical Physics, 2012, 14, 13058.	2.8	15
41	Ultrathin Carbon Nanotube With Single, Double, and Triple Bonds. Physical Review Letters, 2012, 109, 105501.	7.8	8
42	Dunnâ€™s index for cluster tendency assessment of pharmacological data sets. Canadian Journal of Physiology and Pharmacology, 2012, 90, 425-433.	1.4	14
43	Comparison of Combinatorial Clustering Methods on Pharmacological Data Sets Represented by Machine Learning-Selected Real Molecular Descriptors. Journal of Chemical Information and Modeling, 2011, 51, 3036-3049.	5.4	25
44	Anabolic and androgenic activities of 19-nor-testosterone steroids: QSAR study using quantum and physicochemical molecular descriptors. Journal of Steroid Biochemistry and Molecular Biology, 2011, 126, 35-45.	2.5	7
45	Coulomb and Exchange contributions to electronic excitations of benzene aggregates. Chemical Physics Letters, 2011, 502, 271-276.	2.6	5
46	Communication: Accurate determination of side-chain torsion angle Ï‡1 in proteins: Phenylalanine residues. Journal of Chemical Physics, 2011, 134, 061101.	3.0	9
47	Interaction of brassinolide with essential amino acid residues: A theoretical approach. Journal of Molecular Graphics and Modelling, 2010, 28, 604-611.	2.4	2
48	Approximate quantum mechanical method for describing excitations and related properties of finite single-walled carbon nanotubes. Physical Review B, 2010, 81, .	3.2	9
49	Theoretical Study of ImidazoleÂ·Â·Â·NO Complexes. Journal of Physical Chemistry A, 2009, 113, 14595-14605.	2.5	3
50	Molecular modeling of porphyrin-based conjugates and subphthalocyanine aggregates. Journal of Porphyrins and Phthalocyanines, 2009, 13, 494-508.	0.8	2
51	A theoretical approach to the solvation of brassinosteroids. Journal of Molecular Graphics and Modelling, 2009, 27, 600-610.	2.4	6
52	On the unusual²Jcoupling dependence onsyn/antiCHO conformation in 5â€Xâ€furanâ€2â€carboxaldehydes. Magnetic Resonance in Chemistry, 2008, 46, 846-850.	1.9	17
53	Applying pattern recognition methods plus quantum and physicoâ€chemical molecular descriptors to analyze the anabolic activity of structurally diverse steroids. Journal of Computational Chemistry, 2008, 29, 317-333.	3.3	19
54	Chemometric and chemoinformatic analyses of anabolic and androgenic activities of testosterone and dihydrotestosterone analogues. Bioorganic and Medicinal Chemistry, 2008, 16, 6448-6459.	3.0	12

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55	Influence of Density Functionals and Basis Sets on One-Bond Carbonâ^'Carbon NMR Spinâ^'Spin Coupling Constants. Journal of Chemical Theory and Computation, 2008, 4, 448-456.	5.3	40
56	Approximating correlation effects in multiconfigurational self-consistent field calculations of spin-spin coupling constants. Journal of Chemical Physics, 2008, 128, 084108.	3.0	17
57	CNDOL: A fast and reliable method for the calculation of electronic properties of very large systems. Applications to retinal binding pocket in rhodopsin and gas phase porphine. Journal of Chemical Physics, 2007, 127, 145102.	3.0	19
58	Potential energy surfaces and Jahn-Teller effect on CH4â‹¯NO complexes. Journal of Chemical Physics, 2007, 127, 104305.	3.0	11
59	Molecular Structure of Chloro-dodecafluorosubphthalocyanato Boron(III) by Gas-Phase Electron Diffraction and Quantum Chemical Calculations. Journal of Physical Chemistry A, 2007, 111, 4542-4550.	2.5	27
60	Effects of the 3- and 4-Methoxy and Acetamide Substituents and Solvent Environment on the Electronic Properties of N-Substituted 1,8-Naphthalimide Derivatives. Journal of Physical Chemistry A, 2007, 111, 9724-9732.	2.5	24
61	Subphthalocyanine-Fused Dimers and Trimers:Â Synthetic, Electrochemical, and Theoretical Studies. Journal of Organic Chemistry, 2007, 72, 2967-2977.	3.2	41
62	On the molecular electron structure of three phosphinine-containing macrocycles. Journal of Computational Chemistry, 2007, 28, 958-966.	3.3	2
63	Theoretical Karplus relationships for vicinal coupling constants around Ï‡1 in Valine. Chemical Physics Letters, 2007, 442, 119-123.	2.6	16
64	Influence of electronic correlation in monoelectronic density in p-space. Theoretical Chemistry Accounts, 2007, 118, 723-732.	1.4	8
65	Density Functional Theory Study of 14N Isotropic Hyperfine Coupling Constants of Organic Radicals. Journal of Physical Chemistry A, 2006, 110, 13600-13608.	2.5	55
66	Molecular SchrÃ¶dingerâ€“Riccati Calculations: The Potential Energy Curve of the Hydrogen Molecule. Journal of Mathematical Chemistry, 2005, 38, 565-573.	1.5	2
67	Acid-base behavior of triazoleporphyrazines in proton-donating media. Journal of Physical Organic Chemistry, 2005, 18, 329-335.	1.9	9
68	Estimates of non-relativistic atomic and correlation energies. Journal of Physics B: Atomic, Molecular and Optical Physics, 2005, 38, 279-284.	1.5	2
69	Basis set superposition error in MP2 and density-functional theory: A case of methane-nitric oxide association. Journal of Chemical Physics, 2005, 123, 134107.	3.0	31
70	Structural Modulation of the Dipolarâ^'Octupolar Contributions to the NLO Response in Subphthalocyanines. Journal of Physical Chemistry B, 2005, 109, 3800-3806.	2.6	98
71	Theoretical Isotropic Hyperfine Coupling Constants of Third-Row Nuclei (29Si,31P, and33S). Journal of Physical Chemistry A, 2005, 109, 7626-7635.	2.5	45
72	Density Functional Theory Predictions of Isotropic Hyperfine Coupling Constants. Journal of Physical Chemistry A, 2005, 109, 1114-1124.	2.5	102

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73	Theoretical study of low-lying electronic states of BP molecule. Chemical Physics Letters, 2003, 381, 720-724.	2.6	8
74	The Ïƒ-donating and Ï€-accepting properties ofortho-Si(CH3)3phosphinine macrocycles. Heteroatom Chemistry, 2003, 14, 160-169.	0.7	8
75	Polarized basis sets of Slater-type orbitals: H to Ne atoms. Journal of Computational Chemistry, 2003, 24, 859-868.	3.3	62
76	Conformational study of the vinylphosphonic acid and derivatives. International Journal of Quantum Chemistry, 2003, 91, 333-338.	2.0	4
77	Density functional study of the redox processes in subphthalocyanines. International Journal of Quantum Chemistry, 2003, 91, 369-375.	2.0	21
78	DFT study of the electronic structure and Jahn-Teller effect of tetrabromomethane cation. International Journal of Quantum Chemistry, 2003, 91, 414-417.	2.0	2
79	Novel Pushâ^'Pull Phthalocyanines as Targets for Second-Order Nonlinear Applications. Journal of Physical Chemistry A, 2003, 107, 2110-2117.	2.5	51
80	Subphthalocyanines and Subnaphthalocyanines:â€‰ Nonlinear Quasi-Planar Octupolar Systems with Permanent Polarity. Journal of Physical Chemistry B, 2002, 106, 13139-13145.	2.6	60
81	The SchrÃ¶dingerÂ–Riccati equation. The ground-state energy of Be I. Canadian Journal of Physics, 2002, 80, 1053-1057.	1.1	5
82	Molecular Schrï¿½dinger-Riccati calculations. Test for the hydrogen-ion molecule. Theoretical Chemistry Accounts, 2001, 106, 434-438.	1.4	5
83	The axial coordination in subphthalocyanines: Geometrical and electronic aspects. Journal of Porphyrins and Phthalocyanines, 2001, 05, 491-499.	0.8	28
84	A theoretical approach to the influence of the macrocycle conformation on the molecular electronic structure in Mg-porphyrins. Journal of Computer-Aided Molecular Design, 2001, 15, 183-193.	2.9	7
85	A theoretical study of subphthalocyanine and its nitro- and tertbutyl-derivatives. Computational and Theoretical Chemistry, 2001, 537, 223-234.	1.5	31
86	Double- and triple-zeta Slater-type basis sets with common exponents. Theoretical Chemistry Accounts, 2000, 104, 167-171.	1.4	7
87	Molecular modeling of highly peripheral substituted Mg- and Zn-porphyrins. Physical Chemistry Chemical Physics, 2000, 2, 4147-4156.	2.8	13
88	Possible sources of error in the computer simulation of protein structures and interactions. Theoretical and Computational Chemistry, 1999, , 655-663.	0.4	0
89	Electron Affinity of SF6. Advances in Quantum Chemistry, 1997, 28, 189-203.	0.8	9
90	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

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91	Slater Functions for Y to Cd Atoms by the Distance between Subspaces. Journal of Solid State Chemistry, 1995, 116, 275-280.	2.9	5
92	Accurate Roothaan-Hartree-Fock momentum expectation values for ground states of the atoms He to Xe. Chemical Physics Letters, 1995, 236, 616-620.	2.6	9
93	Relativistic corrections to the atomic electron affinities. Physical Review A, 1995, 51, 2616-2618.	2.5	15
94	Numerical Hartree-Fock energies for H–I-1anions. Journal of Physics B: Atomic, Molecular and Optical Physics, 1994, 27, L447-L449.	1.5	5
95	Single-exponent Slater function expansions of the He atom 1s orbital and its isoelectronic series. Chemical Physics Letters, 1993, 207, 270-274.	2.6	7
96	Analytic expressions for one-centrep-space integrals over Slater functions. Journal of Mathematical Chemistry, 1993, 14, 219-229.	1.5	7
97	Application of orbital momentum properties to the analysis of the quality of basis sets. Computational and Theoretical Chemistry, 1993, 287, 39-46.	1.5	3
98	Electron spin resonance and ab initio studies on the cationâ€"semidione interaction. Journal of Molecular Structure, 1992, 269, 163-174.	3.6	2
99	A new procedure to obtain GTO wave functions and to analyze their quality. Computational and Theoretical Chemistry, 1992, 254, 21-29.	1.5	3
100	Jahn-Teller effect and dissociation from the ground state of CF4+. Chemical Physics, 1991, 151, 335-342.	1.9	16
101	Application of the distance between subspaces to the evaluation of wavefunction quality. Computational and Theoretical Chemistry, 1990, 210, 79-84.	1.5	10
102	Quantum chemical applications of the theory of the distance between subspaces. Computational and Theoretical Chemistry, 1989, 184, 1-10.	1.5	11
103	Theoretical approach to the conformational and configurational stability of Î±-sulphinyl carbanions derived from 1,4-oxathiane S-oxides. Journal of the Chemical Society Perkin Transactions II, 1988, , 1573-1577.	0.9	1
104	Two-configuration mc potential energy surface for the reaction of Mg with HF. Chemical Physics, 1986, 101, 55-65.	1.9	14
105	On the interpretation of the electronic structure and ESR spectrum of CH+4. Journal of Molecular Structure, 1986, 142, 323-326.	3.6	3
106	ESR study and ab initio calculations of some methylbenzoates derivatives.. Journal of Molecular Structure, 1986, 142, 427-430.	3.6	5
107	Configurational assignment and conformational study of 1-methylsulfinyl-2-propanol by 1H-NMR and AB initio calculations. Journal of Molecular Structure, 1986, 144, 109-119.	3.6	10
108	RHF potential energy surface for the collinear reaction of Na with HF. Journal of Molecular Structure, 1986, 142, 525-528.	3.6	12

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109	Atomic partitioning of long-range two-center potentials. Computational and Theoretical Chemistry, 1985, 120, 163-174.	1.5	8
110	Theoretical calculations of the hyperfine coupling constants of organic radicals.. Computational and Theoretical Chemistry, 1985, 120, 383-386.	1.5	9
111	Potential energy surface for collinear Mg + FH â†' MgF + H reaction. Computational and Theoretical Chemistry, 1985, 120, 475-478.	1.5	9
112	Electronic structure of CH3OH+. Restricted hartreeâ€"fock calculations of the first two states. Journal of the Chemical Society, Faraday Transactions 2, 1984, 80, 1269-1272.	1.1	1
113	Dissociation of piethanol ion. Computational and Theoretical Chemistry, 1984, 107, 133-138.	1.5	1
114	Ab initio calculations of the potential surface for the 2A1, state of CH4+. Computational and Theoretical Chemistry, 1983, 105, 31-36.	1.5	6
115	Searching conformational analysis of Asp residues through theoretical <scp> ³ J </scp> vicinal coupling constants and Karplus equations. International Journal of Quantum Chemistry, 0, , .	2.0	1