Marco Antonio Chaer Nascimento

List of Publications by Year in Descending Order

73 papers	1,000 citations	20 h-index	26 g-index
77 ext. papers	1,123 ext. citations	3.6 avg, IF	4.84 L-index

#	Paper	IF	Citations
73	The influence of montmorillonite on the flame-retarding properties of intumescent bio-based PLA composites. *Journal of Applied Polymer Science*, **2022**, 139, 52243	2.9	1
72	Ab initio study of structural and electronic properties of lithium fluoride nanotubes. *Journal of Applied Physics*, **2021**, 129, 205102	2.5	0
71	Substituent Effects on the Quantum Interference of Two-Center One-Electron Bonds: [BX] (X = H, F, Cl, CN, OH, CH, and OCH). *Journal of Physical Chemistry A*, **2021**, 125, 4558-4564	2.8	4
70	The Valence-Bond (VB) Model and Its Intimate Relationship to the Symmetric or Permutation Group. *Molecules*, **2021**, 26,	4.8	2
69	Splitting of multiple hydrogen molecules by bioinspired diniobium metal complexes: a DFT study. *Dalton Transactions*, **2021**, 50, 840-849	4.3	2
68	Molecular Photoionization and Photodetachment Cross Sections Based on L(^2) Basis Sets: Theory and Selected Examples. *Progress in Theoretical Chemistry and Physics*, **2021**, 151-179	0.6	1
67	X-ray Photoionization Cross Section Spectra of Water and Ammonia Bonded on Polycyclic Aromatic Hydrocarbons: A Quantum Mechanical Interpretation to the Absorption Spectra on Graphene. *Journal of Physical Chemistry A*, **2020**, 124, 2591-2600	2.8	1
66	Are disulfide bonds resilient to double ionization? Insights from coincidence spectroscopy and calculations.. *RSC Advances*, **2020**, 10, 35039-35048	3.7	
65	Dissociative single and double photoionization of biphenyl (C12H10) by soft X-rays in planetary nebulae. *Monthly Notices of the Royal Astronomical Society*, **2020**, 499, 6066-6083	4.3	1
64	Synergistic Action of Montmorillonite with an Intumescent Formulation: The Impact of the Nature and the Strength of Acidic Sites on the Flame-Retardant Properties of Polypropylene Composites. *Polymers*, **2020**, 12,	4.5	4
63	Three-center two-electron bonds in the boranes B2H6 and B3H8□from the quantum interference perspective. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	3
62	Influence of the zeolite acidity on its synergistic action with a flame-retarding polymeric intumescent formulation. *Journal of Materials Science*, **2020**, 55, 619-630	4.3	5
61	Soft X-ray Chlorine Photolysis on Chlorobenzene Ice: An Experimental and Theoretical Study. *Journal of Physical Chemistry A*, **2019**, 123, 1389-1398	2.8	3
60	One-electron bonds are not "half-bonds". *Physical Chemistry Chemical Physics*, **2019**, 21, 13319-13336	3.6	12
59	Molecular inner-shell photoabsorption/photoionization cross sections at core-valence-separated coupled cluster level: Theory and examples. *Journal of Chemical Physics*, **2019**, 150, 224104	3.9	22
58	Theoretical study of the absolute inner-shell photoionization cross sections of the formic acid and some of its hydrogen-bonded clusters. *Journal of Chemical Physics*, **2019**, 150, 154308	3.9	4
57	Mechanistic Insights into the Formation of Lithium Fluoride Nanotubes. *Chemistry - A European Journal*, **2019**, 25, 5269-5279	4.8	3

56	The consequences of neglecting permutation symmetry in the description of many-electrons systems. *International Journal of Quantum Chemistry*, **2019**, 119, e25765	2.1	9
55	NMR evaluation of montmorillonite d-spacings on the formation of phosphocarbonaceous species in intumescent systems. *Journal of Applied Polymer Science*, **2019**, 136, 48053	2.9	3
54	Lanczos-based equation-of-motion coupled-cluster singles-and-doubles approach to the total photoionization cross section of valence excited states. *Journal of Chemical Physics*, **2019**, 151, 184106	3.9	5
53	Unexpected reversal of stability in strained systems containing one-electron bonds. *Physical Chemistry Chemical Physics*, **2019**, 21, 24984-24992	3.6	9
52	Diboryne Nanostructures Stabilized by Multitopic N-Heterocyclic Carbenes: A Computational Study. *Inorganic Chemistry*, **2018**, 57, 3931-3940	5.1	8
51	Hydrogenated Benzene in Circumstellar Environments: Insights into the Photostability of Super-hydrogenated PAHs. *Astrophysical Journal*, **2018**, 854, 61	4.7	14
50	Time-dependent density functional theory description of total photoabsorption cross sections. *Journal of Chemical Physics*, **2018**, 148, 074104	3.9	11
49	Quantum Interference Contribution to the Dipole Moment of Diatomic Molecules. *Journal of Physical Chemistry A*, **2018**, 122, 1406-1412	2.8	8
48	Doubly and Triply Charged Species Formed from Chlorobenzene Reveal Unusual C-Cl Multiple Bonding. *Journal of the American Chemical Society*, **2018**, 140, 4288-4292	16.4	8
47	Coupled Cluster and Time-Dependent Density Functional Theory Description of Inner Shell Photoabsorption Cross Sections of Molecules. *Journal of Chemical Theory and Computation*, **2018**, 14, 5324-5338	6.4	10
46	The Nature of the Chemical Bond from a Quantum Mechanical Interference Perspective. *ChemistrySelect*, **2017**, 2, 604-619	1.8	17
45	Chemical bonding in the pentagonal-pyramidal benzene dication and analogous isoelectronic hexa-coordinate species. *Computational and Theoretical Chemistry*, **2017**, 1116, 225-233	2	22
44	Paving the Way for the Molecular-Level Design of Adsorbents for Carbon Capture: A Quantum-Chemical Investigation of the Adsorption of CO2 and N2 on Pure-Silica Chabazite. *Journal of Physical Chemistry C*, **2017**, 121, 19314-19320	3.8	5
43	Are One-Electron Bonds Any Different from Standard Two-Electron Covalent Bonds?. *Accounts of Chemical Research*, **2017**, 50, 2264-2272	24.3	27
42	On the metastability of doubly charged homonuclear diatomics. *Physical Chemistry Chemical Physics* , **2017**, 19, 19352-19359	3.6	17
41	Coupled Cluster Study of Photoionization and Photodetachment Cross Sections. *Journal of Chemical Theory and Computation*, **2016**, 12, 4440-59	6.4	14
40	The Nature of the Singlet and Triplet States of Cyclobutadiene as Revealed by Quantum Interference. *ChemPhysChem*, **2016**, 17, 288-95	3.2	18
39	Is There a Quadruple Bond in C2?. *Journal of Chemical Theory and Computation*, **2016**, 12, 2234-41	6.4	38

38	Prediction of Boron-Boron Triple-Bond Polymers Stabilized by Janus-Type Bis(N-heterocyclic) Carbenes. *Chemistry - A European Journal*, **2015**, 21, 7814-9	4.8	9
37	Nature of the chemical bond and origin of the inverted dipole moment in boron fluoride: a generalized valence bond approach. *Journal of Physical Chemistry A*, **2015**, 119, 5335-43	2.8	29
36	The non-covalent nature of the molecular structure of the benzene molecule. *Physical Chemistry Chemical Physics*, **2014**, 16, 11024-30	3.6	22
35	Description of Polar Chemical Bonds from the Quantum Mechanical Interference Perspective. *Journal of Chemical Theory and Computation*, **2014**, 10, 2322-32	6.4	27
34	Interference energy in C-H and C-C bonds of saturated hydrocarbons: dependence on the type of chain and relationship to bond dissociation energy. *Journal of Physical Chemistry A*, **2013**, 117, 4025-34	2.8	20
33	Alkali halide clusters produced by fast ion impact. *Nuclear Instruments & Methods in Physics Research B*, **2012**, 273, 102-104	1.2	3
32	The role of quantum-mechanical interference and quasi-classical effects in conjugated hydrocarbons. *Physical Chemistry Chemical Physics*, **2012**, 14, 5479-88	3.6	19
31	Alkali Halide Nanotubes: Structure and Stability. *Journal of Physical Chemistry C*, **2012**, 116,	3.8	23
30	Does the H+5 hydrogen cluster exist in dense interstellar clouds?. *International Journal of Quantum Chemistry*, **2012**, 112, 3169-3173	2.1	1
29	Effect of the Zeolite Cavity on the Mechanism of Dehydrogenation of Light Alkanes over Gallium-Containing Zeolites. *Journal of Physical Chemistry C*, **2011**, 115, 10104-10113	3.8	24
28	Interference effect and the nature of the pi-bonding in 1,3-butadiene. *Journal of Physical Chemistry A*, **2010**, 114, 8798-805	2.8	21
27	Energy partitioning for generalized product functions: the interference contribution to the energy of generalized valence bond and spin coupled wave functions. *Journal of Chemical Physics*, **2009**, 130, 104102	3.9	41
26	An experimental and theoretical description of the (NH3)n□{NH3□□2O}+ cluster ions produced by fast ion bombardment. *Chemical Physics Letters*, **2009**, 474, 185-189	2.5	1
25	Reformulation in mathematical programming: An application to quantum chemistry. *Discrete Applied Mathematics*, **2009**, 157, 1309-1318	1	9
24	Theoretical and experimental study of negative LiF clusters produced by fast ion impact on a polycrystalline 7LiF target. *Journal of Physical Chemistry A*, **2009**, 113, 15031-40	2.8	14
23	Chemical bonding in the N(2) molecule and the role of the quantum mechanical interference effect. *Journal of Physical Chemistry A*, **2009**, 113, 12541-8	2.8	23
22	Experimental and theoretical studies of (CsI)n Cs+ cluster ions produced by 355 nm laser desorption ionization. *Journal of Physical Chemistry A*, **2008**, 112, 11061-6	2.8	27
21	The nature of the chemical bond. *Journal of the Brazilian Chemical Society*, **2008**, 19,	1.5	16

20	Characterization of (NH3)(n=1-6)NH+ clusters produced by 252Cf fragments impact onto a NH3 condensed target. *Journal of Physical Chemistry A*, **2007**, 111, 8302-7	2.8	7
19	On the calculated first hyperpolarizability of substituted tri-cyclohexadien-2-yl-amines: Novel targets for experimental research. *Computational and Theoretical Chemistry*, **2007**, 811, 337-343		
18	Experimental and theoretical characterization of the Cn=2,16- clusters produced by 337 nm UV laser. *Chemical Physics Letters*, **2007**, 445, 147-151	2.5	13
17	Theoretical study on the dehydrogenation reaction of alkanes catalyzed by zeolites containing nonframework gallium species. *Journal of Physical Chemistry B*, **2006**, 110, 3231-8	3.4	31
16	A density functional study on the effect of the zeolite cavity on its catalytic activity: The dehydrogenation and cracking reactions of isobutane over HZSM-5 and HY zeolites. *Chemical Physics Letters*, **2006**, 418, 368-372	2.5	14
15	Characterization of . *Chemical Physics Letters*, **2006**, 426, 351-356	2.5	16
14	Laser induced formation of CsI ion clusters analyzed by delayed extraction time-of-flight mass spectrometry. *Physical Chemistry Chemical Physics*, **2005**, 7, 1971-6	3.6	8
13	Theoretical study of the dehydrogenation reaction of ethane catalyzed by zeolites containing non-framework gallium species: The 3-step mechanism the 1-step concerted mechanism. *Chemical Physics Letters*, **2005**, 406, 446-451	2.5	37
12	Using an interval branch-and-bound algorithm in the HartreeFock method. *International Journal of Quantum Chemistry*, **2005**, 103, 500-504	2.1	3
11	Ground state of the beryllium atom: Reinvestigation based on a proper independent particle model. *International Journal of Quantum Chemistry*, **2004**, 99, 317-324	2.1	5
10	The dehydrogenation and cracking reactions of isobutane over the ZSM-5 zeolite. *Chemical Physics Letters*, **2003**, 373, 379-384	2.5	30
9	Quantum Mechanics of Many-Electrons Systems and the Theories of Chemical Bond **2003**, 371-405		5
8	Clustering of Hydrogen Molecules around a Molecular Cation: The Li3+(H2)n Clusters (n = 1 6). *Journal of Physical Chemistry A*, **2002**, 106, 551-555	2.8	17
7	A density-functional study of the dehydrogenation reaction of isobutane over zeolites. *Chemical Physics Letters*, **2001**, 338, 67-73	2.5	37
6	A generalized multistructural wave function. *Journal of Chemical Physics*, **1993**, 99, 1207-1214	3.9	39
5	A generalized multi-structural wavefunction. The He+2 molecule as an example. *Chemical Physics Letters*, **1991**, 184, 470-478	2.5	33
4	Photoionization cross sections and dynamic polarizabilities for the lithium atom and positive ion using L2 basis sets and correlated wave functions. *Physical Review A*, **1990**, 42, 6608-6615	2.6	13
3	Calculation of photionization cross-sections and dynamic polarizabilities using square integrable basis sets and correlated wave functions. *Computational and Theoretical Chemistry*, **1985**, 120, 227-240		8

2	The photodetachment cross section of the negative hydrogen ion. *Physical Review A*, **1977**, 16, 1559-1567.	1.6	18
1	Three-centre two-electron bonds from the quantum interference perspective. *Physical Chemistry Chemical Physics*,	3.6	2