

Marco Antonio Chaer Nascimento

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papers

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#	Paper	IF	Citations
73	Energy partitioning for generalized product functions: the interference contribution to the energy of generalized valence bond and spin coupled wave functions. <i>Journal of Chemical Physics</i> , 2009 , 130, 104102	3.9	41
72	A generalized multistructural wave function. <i>Journal of Chemical Physics</i> , 1993 , 99, 1207-1214	3.9	39
71	Is There a Quadruple Bond in C ₂ ?. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 2234-41	6.4	38
70	Theoretical study of the dehydrogenation reaction of ethane catalyzed by zeolites containing non-framework gallium species: The 3-step mechanism vs the 1-step concerted mechanism. <i>Chemical Physics Letters</i> , 2005 , 406, 446-451	2.5	37
69	A density-functional study of the dehydrogenation reaction of isobutane over zeolites. <i>Chemical Physics Letters</i> , 2001 , 338, 67-73	2.5	37
68	A generalized multi-structural wavefunction. The He+2 molecule as an example. <i>Chemical Physics Letters</i> , 1991 , 184, 470-478	2.5	33
67	Theoretical study on the dehydrogenation reaction of alkanes catalyzed by zeolites containing nonframework gallium species. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 3231-8	3.4	31
66	The dehydrogenation and cracking reactions of isobutane over the ZSM-5 zeolite. <i>Chemical Physics Letters</i> , 2003 , 373, 379-384	2.5	30
65	Nature of the chemical bond and origin of the inverted dipole moment in boron fluoride: a generalized valence bond approach. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 5335-43	2.8	29
64	Description of Polar Chemical Bonds from the Quantum Mechanical Interference Perspective. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2322-32	6.4	27
63	Are One-Electron Bonds Any Different from Standard Two-Electron Covalent Bonds?. <i>Accounts of Chemical Research</i> , 2017 , 50, 2264-2272	24.3	27
62	Experimental and theoretical studies of (CsI) _n Cs ⁺ cluster ions produced by 355 nm laser desorption ionization. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 11061-6	2.8	27
61	Effect of the Zeolite Cavity on the Mechanism of Dehydrogenation of Light Alkanes over Gallium-Containing Zeolites. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 10104-10113	3.8	24
60	Alkali Halide Nanotubes: Structure and Stability. <i>Journal of Physical Chemistry C</i> , 2012 , 116,	3.8	23
59	Chemical bonding in the N(2) molecule and the role of the quantum mechanical interference effect. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 12541-8	2.8	23
58	Chemical bonding in the pentagonal-pyramidal benzene dication and analogous isoelectronic hexa-coordinate species. <i>Computational and Theoretical Chemistry</i> , 2017 , 1116, 225-233	2	22
57	Molecular inner-shell photoabsorption/photoionization cross sections at core-valence-separated coupled cluster level: Theory and examples. <i>Journal of Chemical Physics</i> , 2019 , 150, 224104	3.9	22

56	The non-covalent nature of the molecular structure of the benzene molecule. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 11024-30	3.6	22
55	Interference effect and the nature of the pi-bonding in 1,3-butadiene. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 8798-805	2.8	21
54	Interference energy in C-H and C-C bonds of saturated hydrocarbons: dependence on the type of chain and relationship to bond dissociation energy. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 4025-34	2.8	20
53	The role of quantum-mechanical interference and quasi-classical effects in conjugated hydrocarbons. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 5479-88	3.6	19
52	The Nature of the Singlet and Triplet States of Cyclobutadiene as Revealed by Quantum Interference. <i>ChemPhysChem</i> , 2016 , 17, 288-95	3.2	18
51	The photodetachment cross section of the negative hydrogen ion. <i>Physical Review A</i> , 1977 , 16, 1559-1567	2.6	18
50	The Nature of the Chemical Bond from a Quantum Mechanical Interference Perspective. <i>ChemistrySelect</i> , 2017 , 2, 604-619	1.8	17
49	On the metastability of doubly charged homonuclear diatomics. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 19352-19359	3.6	17
48	Clustering of Hydrogen Molecules around a Molecular Cation: The $\text{Li}_3^+(\text{H}_2)_n$ Clusters ($n = 1-6$). <i>Journal of Physical Chemistry A</i> , 2002 , 106, 551-555	2.8	17
47	Characterization of . <i>Chemical Physics Letters</i> , 2006 , 426, 351-356	2.5	16
46	The nature of the chemical bond. <i>Journal of the Brazilian Chemical Society</i> , 2008 , 19,	1.5	16
45	Hydrogenated Benzene in Circumstellar Environments: Insights into the Photostability of Super-hydrogenated PAHs. <i>Astrophysical Journal</i> , 2018 , 854, 61	4.7	14
44	Coupled Cluster Study of Photoionization and Photodetachment Cross Sections. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 4440-59	6.4	14
43	Theoretical and experimental study of negative LiF clusters produced by fast ion impact on a polycrystalline 7LiF target. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 15031-40	2.8	14
42	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. <i>Chemical Physics Letters</i> , 2006 , 418, 368-372	2.5	14
41	Experimental and theoretical characterization of the $\text{C}_n=2,16-$ clusters produced by 337 nm UV laser. <i>Chemical Physics Letters</i> , 2007 , 445, 147-151	2.5	13
40	Photoionization cross sections and dynamic polarizabilities for the lithium atom and positive ion using L2 basis sets and correlated wave functions. <i>Physical Review A</i> , 1990 , 42, 6608-6615	2.6	13
39	One-electron bonds are not "half-bonds". <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 13319-13336	3.6	12

38	Time-dependent density functional theory description of total photoabsorption cross sections. <i>Journal of Chemical Physics</i> , 2018 , 148, 074104	3.9	11
37	Coupled Cluster and Time-Dependent Density Functional Theory Description of Inner Shell Photoabsorption Cross Sections of Molecules. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 5324-5338	6.4	10
36	The consequences of neglecting permutation symmetry in the description of many-electrons systems. <i>International Journal of Quantum Chemistry</i> , 2019 , 119, e25765	2.1	9
35	Prediction of Boron-Boron Triple-Bond Polymers Stabilized by Janus-Type Bis(N-heterocyclic) Carbenes. <i>Chemistry - A European Journal</i> , 2015 , 21, 7814-9	4.8	9
34	Reformulation in mathematical programming: An application to quantum chemistry. <i>Discrete Applied Mathematics</i> , 2009 , 157, 1309-1318	1	9
33	Unexpected reversal of stability in strained systems containing one-electron bonds. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 24984-24992	3.6	9
32	Diboryne Nanostructures Stabilized by Multitopic N-Heterocyclic Carbenes: A Computational Study. <i>Inorganic Chemistry</i> , 2018 , 57, 3931-3940	5.1	8
31	Quantum Interference Contribution to the Dipole Moment of Diatomic Molecules. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 1406-1412	2.8	8
30	Doubly and Triply Charged Species Formed from Chlorobenzene Reveal Unusual C-Cl Multiple Bonding. <i>Journal of the American Chemical Society</i> , 2018 , 140, 4288-4292	16.4	8
29	Laser induced formation of CsI ion clusters analyzed by delayed extraction time-of-flight mass spectrometry. <i>Physical Chemistry Chemical Physics</i> , 2005 , 7, 1971-6	3.6	8
28	Calculation of photionization cross-sections and dynamic polarizabilities using square integrable basis sets and correlated wave functions. <i>Computational and Theoretical Chemistry</i> , 1985 , 120, 227-240		8
27	Characterization of (NH ₃)(n=1-6)NH ⁺ clusters produced by 252Cf fragments impact onto a NH ₃ condensed target. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 8302-7	2.8	7
26	Paving the Way for the Molecular-Level Design of Adsorbents for Carbon Capture: A Quantum-Chemical Investigation of the Adsorption of CO ₂ and N ₂ on Pure-Silica Chabazite. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 19314-19320	3.8	5
25	Ground state of the beryllium atom: Reinvestigation based on a proper independent particle model. <i>International Journal of Quantum Chemistry</i> , 2004 , 99, 317-324	2.1	5
24	Quantum Mechanics of Many-Electrons Systems and the Theories of Chemical Bond 2003 , 371-405		5
23	Lanczos-based equation-of-motion coupled-cluster singles-and-doubles approach to the total photoionization cross section of valence excited states. <i>Journal of Chemical Physics</i> , 2019 , 151, 184106	3.9	5
22	Influence of the zeolite acidity on its synergistic action with a flame-retarding polymeric intumescent formulation. <i>Journal of Materials Science</i> , 2020 , 55, 619-630	4.3	5
21	Theoretical study of the absolute inner-shell photoionization cross sections of the formic acid and some of its hydrogen-bonded clusters. <i>Journal of Chemical Physics</i> , 2019 , 150, 154308	3.9	4

20	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. <i>Polymers</i> , 2020 , 12,	4.5	4
19	Substituent Effects on the Quantum Interference of Two-Center One-Electron Bonds: [BX] (X = H, F, Cl, CN, OH, CH, and OCH). <i>Journal of Physical Chemistry A</i> , 2021 , 125, 4558-4564	2.8	4
18	Soft X-ray Chlorine Photolysis on Chlorobenzene Ice: An Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 1389-1398	2.8	3
17	Mechanistic Insights into the Formation of Lithium Fluoride Nanotubes. <i>Chemistry - A European Journal</i> , 2019 , 25, 5269-5279	4.8	3
16	NMR evaluation of montmorillonite d-spacings on the formation of phosphocarbonaceous species in intumescent systems. <i>Journal of Applied Polymer Science</i> , 2019 , 136, 48053	2.9	3
15	Alkali halide clusters produced by fast ion impact. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2012 , 273, 102-104	1.2	3
14	Using an interval branch-and-bound algorithm in the Hartree-Fock method. <i>International Journal of Quantum Chemistry</i> , 2005 , 103, 500-504	2.1	3
13	Three-center two-electron bonds in the boranes B ₂ H ₆ and B ₃ H ₈ from the quantum interference perspective. <i>Theoretical Chemistry Accounts</i> , 2020 , 139, 1	1.9	3
12	The Valence-Bond (VB) Model and Its Intimate Relationship to the Symmetric or Permutation Group. <i>Molecules</i> , 2021 , 26,	4.8	2
11	Splitting of multiple hydrogen molecules by bioinspired diniobium metal complexes: a DFT study. <i>Dalton Transactions</i> , 2021 , 50, 840-849	4.3	2
10	Three-centre two-electron bonds from the quantum interference perspective. <i>Physical Chemistry Chemical Physics</i> ,	3.6	2
9	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. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 2591-2600	2.8	1
8	Does the H ₅ hydrogen cluster exist in dense interstellar clouds?. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 3169-3173	2.1	1
7	An experimental and theoretical description of the (NH ₃) _n {(NH ₃) _m H ₂ O} ⁺ cluster ions produced by fast ion bombardment. <i>Chemical Physics Letters</i> , 2009 , 474, 185-189	2.5	1
6	Dissociative single and double photoionization of biphenyl (C ₁₂ H ₁₀) by soft X-rays in planetary nebulae. <i>Monthly Notices of the Royal Astronomical Society</i> , 2020 , 499, 6066-6083	4.3	1
5	Molecular Photoionization and Photodetachment Cross Sections Based on L ^(^2) Basis Sets: Theory and Selected Examples. <i>Progress in Theoretical Chemistry and Physics</i> , 2021 , 151-179	0.6	1
4	The influence of montmorillonite on the flame-retarding properties of intumescent bio-based PLA composites. <i>Journal of Applied Polymer Science</i> , 2022 , 139, 52243	2.9	1
3	Ab initio study of structural and electronic properties of lithium fluoride nanotubes. <i>Journal of Applied Physics</i> , 2021 , 129, 205102	2.5	0

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