

Alexandre Braga Rocha

List of Publications by Year in descending order

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106
papers

1,372
citations

448610

19
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511568

30
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106
all docs

106
docs citations

106
times ranked

1562
citing authors

#	ARTICLE	IF	CITATIONS
1	Microsolvation effect on chlorination reaction of simple alcohols. International Journal of Chemical Kinetics, 2022, 54, 381-388.	1.0	1
2	Glycerol chlorination reaction mechanism. International Journal of Chemical Kinetics, 2021, 53, 369-378.	1.0	2
3	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.	0.2	5
4	Evidence of ultrafast dissociation in the CHCl ₃ molecule. Journal of Physics B: Atomic, Molecular and Optical Physics, 2021, 54, 015202.	0.6	3
5	Electron-Molecule Collisions with Explicit Ro-Vibrational Resolution at MRCI Level and Using Even Tempered Basis Sets. Journal of Chemical Physics, 2021, 155, 194110.	1.2	1
6	Insights into the Phosphate Species on Niobia Treated with H ₃ PO ₄ . Catalysis Letters, 2020, 150, 1496-1504.	1.4	3
7	Structure, Stability, and Spectroscopic Properties of Small Acetonitrile Cation Clusters. Journal of Physical Chemistry A, 2020, 124, 6845-6855.	1.1	6
8	Atomic and molecular Auger decay in CHCl ₃ molecule. Journal of Physics: Conference Series, 2020, 1412, 122013.	0.3	0
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. Journal of Physical Chemistry A, 2020, 124, 2591-2600.	1.1	4
10	Rotational spectrum simulations of asymmetric tops in an astrochemical context. Journal of Molecular Modeling, 2020, 26, 278.	0.8	2
11	Inner-valence Auger decay in chloroform after Cl 2p ionization. Nuclear Instruments & Methods in Physics Research B, 2019, 461, 133-136.	0.6	2
12	Acrylic acid hydrodeoxygenation reaction mechanism over molybdenum carbide studied by DFT calculations. Journal of Molecular Modeling, 2019, 25, 309.	0.8	2
13	Ultrafast dissociation of CD ₂ Cl ₂ and CH ₂ Cl ₂ . AIP Conference Proceedings, 2019, , .	0.3	0
14	Soft X-ray Chlorine Photolysis on Chlorobenzene Ice: An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2019, 123, 1389-1398.	1.1	4
15	Molecular inner-shell photoabsorption/photoionization cross sections at core-valence-separated coupled cluster level: Theory and examples. Journal of Chemical Physics, 2019, 150, 224104.	1.2	33
16	Generalized oscillator strengths of carbon disulfide calculated by multireference configuration interaction. Journal of Chemical Physics, 2019, 150, 174116.	1.2	11
17	Ab initio study of diffusion of hydrogen, silver and lithium in PbS and Ag ₂ S. Computational Materials Science, 2019, 166, 75-81.	1.4	9
18	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.	1.2	7

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19	Experimental and theoretical results of resonant and normal Auger decay in dichloromethane. <i>European Physical Journal D</i> , 2019, 73, 1.	0.6	4
20	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.	1.2	12
21	Transitions energies, optical oscillator strengths and partial potential energy surfaces of inner-shell states of water clusters. <i>Chemical Physics</i> , 2018, 508, 26-33.	0.9	11
22	Time-dependent density functional theory description of total photoabsorption cross sections. <i>Journal of Chemical Physics</i> , 2018, 148, 074104.	1.2	14
23	Fragment and cluster ions from gaseous and condensed pyridine produced under electron impact. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25762-25771.	1.3	6
24	Atomic versus molecular Auger decay in CH ₂ Cl ₂ and CD ₂ Cl ₂ molecules. <i>Journal of Chemical Physics</i> , 2018, 149, 054303.	1.2	17
25	Fragmentation of Valence and Carbon Core Excited and Ionized CH ₂ FCF ₃ Molecule. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9755-9760.	1.1	11
26	High-Resolution Near-Edge X-ray Absorption Fine Structure Study of Condensed Polyacenes. <i>Journal of Physical Chemistry C</i> , 2018, 122, 28692-28701.	1.5	9
27	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.	2.3	13
28	Synthesis, characterization and biological activity of gallium(III) complexes with non-symmetrical NO-donor Schiff bases. <i>Polyhedron</i> , 2017, 123, 480-489.	1.0	5
29	Fragmentation of Valence and Core "Shell (Cl 2p) Excited C ₂ Cl ₄ Molecule. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4233-4241.	1.1	4
30	Production of the Q2 doubly excited states of the hydrogen molecule by electron impact in a single step. <i>European Physical Journal D</i> , 2017, 71, 1.	0.6	1
31	Hydrodeoxygenation of acrylic acid using Mo ₂ C/Al ₂ O ₃ . <i>Applied Catalysis A: General</i> , 2017, 531, 69-78.	2.2	22
32	Catalytic promiscuity of mononuclear copper(II) complexes in mild conditions: Catechol and cyclohexane oxidations. <i>Polyhedron</i> , 2017, 123, 293-304.	1.0	13
33	Additive Driven Increase in Donor " Acceptor Copolymer Coupling Studied by X-ray Resonant Photoemission. <i>Journal of Physical Chemistry C</i> , 2017, 121, 25187-25194.	1.5	9
34	Breaking the disulfide chemical bond using high energy photons: the dimethyl disulfide and methyl propyl disulfide molecules. <i>RSC Advances</i> , 2017, 7, 36525-36532.	1.7	12
35	Acidity enhancement of niobia by sulfation: An experimental and DFT study. <i>Materials Chemistry and Physics</i> , 2017, 186, 138-145.	2.0	8
36	Electronic and structural properties in thermally annealed PSiF-DBT:PC71BM blends for organic photovoltaics. <i>Thin Solid Films</i> , 2016, 615, 165-170.	0.8	11

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55	Fragmentation of CHClF_2 molecule by electron impact investigated using a time-delayed spectroscopic technique. <i>Physical Review A</i> , 2012, 86, . $\frac{14}{2} \times 15 = 105$	1.0	24
56	Measurements of Energy Distribution of Molecular Ions and their Fragments Produced by Electron Impact with a New Spectroscopic Technique. <i>Journal of Physics: Conference Series</i> , 2012, 388, 052001.	0.3	0
57	Identification of the CHClF_2 molecule fragmentation paths by electron impact. <i>Journal of Physics: Conference Series</i> , 2012, 388, 052005.	0.3	1
58	Fragmentation of the CH_2Cl_2 molecule by attosecond proton beams and synchrotron radiation. <i>Journal of Physics: Conference Series</i> , 2012, 388, 102025.	0.3	0
59	Ab Initio Study of Reaction Pathways Related to Initial Steps of Thermal Decomposition of the Layered Double Hydroxide Compounds. <i>Journal of Physical Chemistry C</i> , 2012, 116, 13679-13687.	1.5	32
60	On the nature of inhibition performance of imidazole on iron surface. <i>Corrosion Science</i> , 2012, 57, 254-259.	3.0	55
61	Comparative Structural, thermodynamic and electronic analyses of ZnAlAn ⁺ hydrotalcite-like compounds ($\text{An}^+ = \text{Cl}^+, \text{F}^+, \text{Br}^+, \text{OH}^+, \text{CO}_3^{2-}$ or NO_3^-): An ab initio study. <i>Applied Clay Science</i> , 2012, 56, 16-22.	2.6	131
62	Core level (S 2p) excitation and fragmentation of the dimethyl sulfide and dimethyldisulfide molecules. <i>Journal of Chemical Physics</i> , 2012, 136, 144307.	1.2	18
63	Synthesis of Niobium Carbonitride by Thermal Decomposition of Guanidine Oxaloniobate and Its Application to the Hydrodesulfurization of Dibenzothiophene. <i>Topics in Catalysis</i> , 2012, 55, 910-921.	1.3	9
64	Positive molecular ions and ion-neutral complexes in the gas phase: Structure and stability of $\text{C}_2\text{H}_4\text{O}_2^+$ and $\text{C}_2\text{H}_4\text{O}_2^{2+}$ isomers. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3303-3311.	1.0	7
65	Potential curves for inner-shell states of CO calculated at multiconfigurational self-consistent field level. <i>Journal of Chemical Physics</i> , 2011, 134, 024107.	1.2	29
66	Ab Initio Simulation of Changes in Geometry, Electronic Structure, and Gibbs Free Energy Caused by Dehydration of Hydrotalcites Containing Cl^+ and CO_3^{2-} Counteranions. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3531-3537.	1.2	51
67	Photodissociation of methyl formate in circumstellar environment: stability under soft X-rays. <i>Monthly Notices of the Royal Astronomical Society</i> , 2011, 417, 2631-2641.	1.6	23
68	Transition energies and oscillator strength calculated for d-d symmetry-forbidden electronic transition for Cu ⁺ impurities in sodium fluoride host lattice. <i>Chemical Physics</i> , 2011, 389, 102-106.	0.9	6
69	Fragmentation of the CH_2Cl_2 molecule by proton impact and VUV photons. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2011, 44, 165205.	0.6	21
70	The problem of hole localization in inner-shell states of N ₂ and CO ₂ revisited with complete active space self-consistent field approach. <i>Journal of Chemical Physics</i> , 2011, 135, 224112.	1.2	10
71	Benzene adsorption on Mo ₂ C: A theoretical and experimental study. <i>Applied Catalysis A: General</i> , 2010, 379, 54-60.	2.2	43
72	Cross-section measurements for the fragmentation of CHClF_2 by electron impact. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2010, 43, 105203.	0.6	13

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73	Structural Model Proposition and Thermodynamic and Vibrational Analysis of Hydrotalcite-Like Compounds by DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2010, 114, 14133-14140.	1.5	78
74	Theoretical Investigation on the Stability of Negatively Charged Formic Acid Clusters. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6917-6926.	1.1	8
75	Intensity of σ 's symmetry-forbidden electronic transition for Cu ⁺ impurity in sodium chloride. <i>Chemical Physics Letters</i> , 2009, 483, 72-76.	1.2	4
76	DFT calculation of EPR parameters of antisite defect in gallium arsenide. <i>Chemical Physics Letters</i> , 2008, 453, 188-191.	1.2	11
77	Theoretical Investigation on the Stability of Ionic Formic Acid Clusters. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13382-13392.	1.1	14
78	Structural and Energetic Analysis of $Mg_{2-x}M_1(OH)_2$ (M = Zn, Cu or Ca) Brucite-Like Compounds by DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2008, 112, 10681-10687.	1.5	28
79	Negative atomic halogens incident on argon and molecular nitrogen: electron detachment studies. <i>Journal of Physics: Conference Series</i> , 2007, 88, 012024.	0.3	1
80	Intensity of σ 'd Symmetry-Forbidden Electronic Transition in Cr(CO) ₆ . <i>Journal of Physical Chemistry A</i> , 2007, 111, 4711-4713.	1.1	10
81	Experimental and theoretical study of S 2p and C 1s spectroscopy in CS ₂ . <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2007, 156-158, 158-163.	0.8	4
82	Experimental and theoretical study of S 2p and C 1s generalized oscillator strengths in CS ₂ . <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2007, 155, 21-27.	0.8	3
83	Characterization by ²⁷ Al NMR, X-ray Absorption Spectroscopy, and Density Functional Theory Techniques of the Species Responsible for Benzene Hydrogenation in Y Zeolite-Supported Carburized Molybdenum Catalysts. <i>Journal of Physical Chemistry B</i> , 2006, 110, 15803-15811.	1.2	12
84	Double ionization of atoms by ion impact: two-step models. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2006, 39, 1751-1761.	0.6	16
85	Theoretical investigations on the vibronic coupling between the electronic states S ₀ and S ₁ of formic acid including the photodissociation at 248nm. <i>Chemical Physics Letters</i> , 2005, 407, 166-170.	1.2	10
86	Theoretical investigations on valence vibronic transitions. <i>Brazilian Journal of Physics</i> , 2005, 35, 971-980.	0.7	11
87	Young-type interference pattern in molecular inner-shell excitations by electron impact. <i>Physical Review A</i> , 2005, 72, .	1.0	7
88	On the Conformational Memory in the Photodissociation of Formic Acid. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2836-2839.	1.1	18
89	Collisional electron detachment of atomic anions by noble gases: universal behavior at intermediate velocities. <i>Brazilian Journal of Physics</i> , 2004, 34, 825-828.	0.7	3
90	Absolute electron detachment cross sections of atomic anions of the second and third periods incident on noble gases. <i>Physical Review A</i> , 2004, 69, .	1.0	19

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91	Generalized oscillator strength for core excitations of nitrous oxide. <i>Chemical Physics</i> , 2004, 299, 83-88.	0.9	9
92	Forbidden transitions in benzene. <i>Computational and Theoretical Chemistry</i> , 2003, 621, 99-105.	1.5	19
93	Mixed-oxide formation during preparation of alumina-supported zirconia: an EXAFS and DFT study. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 3811-3817.	1.3	20
94	Laser interaction with a pair of two-dimensional coupled quantum dots. <i>Journal of Applied Physics</i> , 2003, 94, 2579-2584.	1.1	8
95	Contributions to the generalized oscillator strength for the inner-shell C 1s π^* transition in CO ₂ from the vibronic coupling mechanism. <i>Physical Review A</i> , 2002, 66, .	1.0	8
96	Direct Investigation of the Validity of Vertical Approximation in the Calculation of Transition Moment Matrix Elements: π^* Transition in Methyl Formate. <i>Journal of Physical Chemistry A</i> , 2002, 106, 181-183.	1.1	18
97	Generalized oscillator strengths for C 1s excitation of acetylene and ethylene. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2002, 123, 303-314.	0.8	17
98	Generalized oscillator strength profiles for inner shell excitation of CO ₂ derived from variable angle electron energy loss spectroscopy. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2001, 114-116, 93-97.	0.8	9
99	Intensity of the π^* symmetry-forbidden electronic transition in acetone by direct vibronic coupling mechanism. <i>Chemical Physics Letters</i> , 2001, 337, 331-334.	1.2	15
100	Isotopic effects in inner-shell spectrum of methane: a theoretical study. <i>Computational and Theoretical Chemistry</i> , 2001, 539, 145-148.	1.5	8
101	Vibronic coupling for H ₂ CO and CO ₂ . <i>Chemical Physics</i> , 2000, 253, 51-57.	0.9	24
102	Explicit core-hole localization and relaxation effects in the calculation of inner-shell spectrum of C ₂ H ₄ . <i>Journal of Chemical Physics</i> , 2000, 113, 7971-7975.	1.2	8
103	Experimental and theoretical study of generalized oscillator strengths for C 1s and O 1s excitations in CO ₂ . <i>Physical Review A</i> , 2000, 61, .	1.0	30
104	Inner-shell excitations of water molecule. <i>Chemical Physics</i> , 1999, 243, 9-15.	0.9	10
105	Optical and generalized oscillator strengths for the B ₁ π^* , C ₁ π^* , and E ₁ π^* vibronic bands in the CO molecule. <i>Physical Review A</i> , 1998, 57, 4394-4400.	1.0	25
106	Fano-Feshbach Formalism Applied to the Calculation of Autoionization Widths through Analytic Continuation. <i>Journal of Chemical Physics</i> , 0, , .	1.2	0