Alexandre Braga Rocha

List of Publications by Year
in descending order

106 papers	1,372 citations	394390 19 h-index	454934 30 g-index
106 all docs	106 docs citations	106 times ranked	1430 citing authors

#	Article	IF	Citations
1	Microsolvation effect on chlorination reaction of simple alcohols. International Journal of Chemical Kinetics, 2022, 54, 381-388.	1.6	1
2	Glycerol chlorination reaction mechanism. International Journal of Chemical Kinetics, 2021, 53, 369-378.	1.6	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 CHCl₃ molecule. Journal of Physics B: Atomic, Molecular and Optical Physics, 2021, 54, 015202.	1.5	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.	3.0	1
6	Insights into the Phosphate Species on Niobia Treated with H3PO4. Catalysis Letters, 2020, 150, 1496-1504.	2.6	3
7	Structure, Stability, and Spectroscopic Properties of Small Acetonitrile Cation Clusters. Journal of Physical Chemistry A, 2020, 124, 6845-6855.	2.5	6
8	Atomic and molecular Auger decay in CHCl3 molecule. Journal of Physics: Conference Series, 2020, 1412, 122013.	0.4	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.	2.5	4
10	Rotational spectrum simulations of asymmetric tops in an astrochemical context. Journal of Molecular Modeling, 2020, 26, 278.	1.8	2
11	Inner-valence Auger decay in chloroform after Cl 2p ionization. Nuclear Instruments & Methods in Physics Research B, 2019, 461, 133-136.	1.4	2
12	Acrylic acid hydrodeoxygenation reaction mechanism over molybdenum carbide studied by DFT calculations. Journal of Molecular Modeling, 2019, 25, 309.	1.8	2
13	Ultrafast dissociation of CD2Cl2 and CH2Cl2. AIP Conference Proceedings, 2019, , .	0.4	0
14	Soft X-ray Chlorine Photolysis on Chlorobenzene Ice: An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2019, 123, 1389-1398.	2.5	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.	3.0	33
16	Generalized oscillator strengths of carbon disulfide calculated by multireference configuration interaction. Journal of Chemical Physics, 2019, 150, 174116.	3.0	11
17	Ab initio study of diffusion of hydrogen, silver and lithium in PbS and Ag2S. Computational Materials Science, 2019, 166, 75-81.	3.0	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.	3.0	7

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19	Experimental and theoretical results of resonant and normal Auger decay in dichloromethane. European Physical Journal D, 2019, 73, 1.	1.3	4
20	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.	3.0	12
21	Transitions energies, optical oscillator strengths and partial potential energy surfaces of inner-shell states of water clusters. Chemical Physics, 2018, 508, 26-33.	1.9	11
22	Time-dependent density functional theory description of total photoabsorption cross sections. Journal of Chemical Physics, 2018, 148, 074104.	3.0	14
23	Fragment and cluster ions from gaseous and condensed pyridine produced under electron impact. Physical Chemistry Chemical Physics, 2018, 20, 25762-25771.	2.8	6
24	Atomic versus molecular Auger decay in CH2Cl2 and CD2Cl2 molecules. Journal of Chemical Physics, 2018, 149, 054303.	3.0	17
25	Fragmentation of Valence and Carbon Core Excited and Ionized CH₂FCF₃ Molecule. Journal of Physical Chemistry A, 2018, 122, 9755-9760.	2.5	11
26	High-Resolution Near-Edge X-ray Absorption Fine Structure Study of Condensed Polyacenes. Journal of Physical Chemistry C, 2018, 122, 28692-28701.	3.1	9
27	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.	5.3	13
28	Synthesis, characterization and biological activity of gallium(III) complexes with non-symmetrical NO-donor Schiff bases. Polyhedron, 2017, 123, 480-489.	2.2	5
29	Fragmentation of Valence and Coreâ€"Shell (Cl 2p) Excited C₂Cl₄ Molecule. Journal of Physical Chemistry A, 2017, 121, 4233-4241.	2.5	4
30	Production of the Q2 doubly excited states of the hydrogen molecule by electron impact in a single step. European Physical Journal D, 2017, 71, 1.	1.3	1
31	Hydrodeoxygenation of acrylic acid using Mo2C/Al2O3. Applied Catalysis A: General, 2017, 531, 69-78.	4.3	22
32	Catalytic promiscuity of mononuclear copper(II) complexes in mild conditions: Catechol and cyclohexane oxidations. Polyhedron, 2017, 123, 293-304.	2.2	13
33	Additive Driven Increase in Donorâ€"Acceptor Copolymer Coupling Studied by X-ray Resonant Photoemission. Journal of Physical Chemistry C, 2017, 121, 25187-25194.	3.1	9
34	Breaking the disulfide chemical bond using high energy photons: the dimethyl disulfide and methyl propyl disulfide molecules. RSC Advances, 2017, 7, 36525-36532.	3.6	12
35	Acidity enhancement of niobia by sulfation: An experimental and DFT study. Materials Chemistry and Physics, 2017, 186, 138-145.	4.0	8
36	Electronic and structural properties in thermally annealed PSiF-DBT:PC71BM blends for organic photovoltaics. Thin Solid Films, 2016, 615, 165-170.	1.8	11

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37	VUV and soft x-ray ionization of a plant volatile: Vanillin (C8H8O3). Journal of Chemical Physics, 2016, 144, 114305.	3.0	8
38	Isomer distribution in Î±-Keggin structures [XW12âˆ’nVnO40]âˆ’(q+n) XÂ=ÂSi, P (0Ââ‰ÂnÂâ‰Â4): A DFT study of free energy and vibrational spectra. Comptes Rendus Chimie, 2016, 19, 1352-1362.	0.5	2
39	Kinetic Energy Release of the Singly and Doubly Charged Methylene Chloride Molecule: The Role of Fast Dissociation. Journal of Physical Chemistry A, 2016, 120, 6728-6737.	2.5	13
40	Coupled Cluster Study of Photoionization and Photodetachment Cross Sections. Journal of Chemical Theory and Computation, 2016, 12, 4440-4459.	5.3	21
41	Symmetry forbidden vibronic transitions near the S K edge excitation of the SF6 molecule. Journal of Physics: Conference Series, 2015, 635, 112026.	0.4	0
42	Strong Selectivity in Symmetry forbidden vibronic transitions in Deep Core Ionic Photofragmentation of the SF6 molecule. International Journal of Mass Spectrometry, 2015, 388, 9-16.	1.5	6
43	Potential energy curves and generalized oscillator strength for doubly excited states of hydrogen molecule. Journal of Physics B: Atomic, Molecular and Optical Physics, 2015, 48, 185104.	1.5	4
44	Electron-detachment cross section for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi>CN</mml:mi><mml:mo>â^’</mml:mo></mml:msup></mm xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msubsup><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn><mml:mo>â^’</mml:mo></mml:msubsup></mml:math>incident on N<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>at intermediate velocities. Physical Review A, 2014, 89,	2.5	4
45	Investigation of hydrogen occlusion by molybdenum carbide. Applied Catalysis A: General, 2014, 469, 139-145.	4.3	13
46	Charge Transfer Dynamics and Molecular Orientation Probed by Core Electron Spectroscopies on thermal-annealed Polysilafluorene Derivative: Experimental and Theoretical Approaches. Journal of Physical Chemistry C, 2014, 118, 23863-23873.	3.1	30
47	Spin-orbit splitting for inner-shell 2p states. Journal of Molecular Modeling, 2014, 20, 2355.	1.8	5
48	Reply to comment on the A.B. Rochaâ€™s reply to second comment on the paper On the nature of inhibition performance of imidazole on iron surface. Corrosion Science, 2014, 79, 221-223.	6.6	0
49	Theoretical and experimental investigation on the stability of C=1â€“6Hâˆ’ and C=1â€“4H+ clusters. Chemical Physics, 2013, 410, 109-117.	1.9	10
50	Reply to comments on the paper â€œOn the nature of inhibition performance of imidazole on iron surfaceâ€•by J.O. Mendes, E.C. da Silva, A.B. Rocha. Corrosion Science, 2013, 70, 298-300.	6.6	2
51	Site-selective photofragmentation of chlorinated polymeric films observed around the chlorine K-edge. Chemical Physics, 2013, 415, 145-149.	1.9	1
52	Reply to comments on the paper â€œOn the nature of inhibition performance of imidazole on iron surfaceâ€•by J.O. Mendes, E.C. da Silva, A.B. Rocha. Corrosion Science, 2013, 68, 290-291.	6.6	4
53	Transition energy and potential energy curves for ionized inner-shell states of CO, O2 and N2 calculated by several inner-shell multiconfigurational approaches. Journal of Molecular Modeling, 2013, 19, 2027-2033.	1.8	11
54	Electron scattering from trans 1,3-butadiene molecule: cross-sections, oscillator strength and VUV photoabsorption cross-sections. European Physical Journal D, 2013, 67, 1.	1.3	3

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55	Fragmentation of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mrow /><mml:mrow><mml:mn>14</mml:mn><mml:mo>,</mml:mo><mml:mn>15</mml:mn></mml:mrow></mml:msup></mml:math>N<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>by electron impact investigated using a time-delayed spectroscopic technique. Physical Review A, 2012, 86, .	2.5	24
56	Measurements of Energy Distribution of Molecular Ions and their Fragments Produced by Electron Impact with a New Spectroscopic Technique. Journal of Physics: Conference Series, 2012, 388, 052001.	0.4	0
57	Identification of the CHClF₂molecule fragmentation paths by electron impact. Journal of Physics: Conference Series, 2012, 388, 052005.	0.4	1
58	Fragmentation of the CH2Cl2molecule by attosecond proton beams and synchrotron radiation. Journal of Physics: Conference Series, 2012, 388, 102025.	0.4	0
59	Ab Initio Study of Reaction Pathways Related to Initial Steps of Thermal Decomposition of the Layered Double Hydroxide Compounds. Journal of Physical Chemistry C, 2012, 116, 13679-13687.	3.1	32
60	On the nature of inhibition performance of imidazole on iron surface. Corrosion Science, 2012, 57, 254-259.	6.6	55
61	Comparative Structural, thermodynamic and electronic analyses of ZnAlAnâˆ’ hydrotalcite-like compounds (Anâˆ’Clâˆ’, Fâˆ’, Brâˆ’, OHâˆ’, CO32âˆ’ or NO3âˆ’): An ab initio study. Applied Clay Science, 2012, 56, 16-22.	5.2	131
62	Core level (S 2p) excitation and fragmentation of the dimethyl sulfide and dimethyldisulfide molecules. Journal of Chemical Physics, 2012, 136, 144307.	3.0	18
63	Synthesis of Niobium Carbonitride by Thermal Decomposition of Guanidine Oxaloniobate and Its Application to the Hydrodesulfurization of Dibenzothiophene. Topics in Catalysis, 2012, 55, 910-921.	2.8	9
64	Positive molecular ions and ionâ€neutral complexes in the gas phase: Structure and stability of C₂H₄O₂^{+Â·} and C₂H₄O₂²⁺ isomers. International Journal of Quantum Chemistry, 2012, 112, 3303-3311.	2.0	7
65	Potential curves for inner-shell states of CO calculated at multiconfigurational self-consistent field level. Journal of Chemical Physics, 2011, 134, 024107.	3.0	29
66	Ab Initio Simulation of Changes in Geometry, Electronic Structure, and Gibbs Free Energy Caused by Dehydration of Hydrotalcites Containing Cl^{âˆ’}and CO₃^{2âˆ’}Counteranions. Journal of Physical Chemistry B, 2011, 115, 3531-3537.	2.6	51
67	Photodissociation of methyl formate in circumstellar environment: stability under soft X-rays. Monthly Notices of the Royal Astronomical Society, 2011, 417, 2631-2641.	4.4	23
68	Transition energies and oscillator strength calculated for dâ€“s symmetry-forbidden electronic transition for Cu+ impurities in sodium fluoride host lattice. Chemical Physics, 2011, 389, 102-106.	1.9	6
69	Fragmentation of the CH₂Cl₂molecule by proton impact and VUV photons. Journal of Physics B: Atomic, Molecular and Optical Physics, 2011, 44, 165205.	1.5	21
70	The problem of hole localization in inner-shell states of N2 and CO2 revisited with complete active space self-consistent field approach. Journal of Chemical Physics, 2011, 135, 224112.	3.0	10
71	Benzene adsorption on Mo2C: A theoretical and experimental study. Applied Catalysis A: General, 2010, 379, 54-60.	4.3	43
72	Cross-section measurements for the fragmentation of CHClF₂by electron impact. Journal of Physics B: Atomic, Molecular and Optical Physics, 2010, 43, 105203.	1.5	13

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73	Structural Model Proposition and Thermodynamic and Vibrational Analysis of Hydrotalcite-Like Compounds by DFT Calculations. Journal of Physical Chemistry C, 2010, 114, 14133-14140.	3.1	78
74	Theoretical Investigation on the Stability of Negatively Charged Formic Acid Clusters. Journal of Physical Chemistry A, 2010, 114, 6917-6926.	2.5	8
75	Intensity of dâ€“s symmetry-forbidden electronic transition for Cu+ impurity in sodium chloride. Chemical Physics Letters, 2009, 483, 72-76.	2.6	4
76	DFT calculation of EPR parameters of antisite defect in gallium arsenide. Chemical Physics Letters, 2008, 453, 188-191.	2.6	11
77	Theoretical Investigation on the Stability of Ionic Formic Acid Clusters. Journal of Physical Chemistry A, 2008, 112, 13382-13392.	2.5	14
78	Structural and Energetic Analysis of Mg_xM_{1â^'x}(OH)₂ (M = Zn, Cu or Ca) Brucite-Like Compounds by DFT Calculations. Journal of Physical Chemistry C, 2008, 112, 10681-10687.	3.1	28
79	Negative atomic halogens incident on argon and molecular nitrogen: electron detachment studies. Journal of Physics: Conference Series, 2007, 88, 012024.	0.4	1
80	Intensity of dâ^'d Symmetry-Forbidden Electronic Transition in Cr(CO)6. Journal of Physical Chemistry A, 2007, 111, 4711-4713.	2.5	10
81	Experimental and theoretical study of S 2p and C 1s spectroscopy in CS2. Journal of Electron Spectroscopy and Related Phenomena, 2007, 156-158, 158-163.	1.7	4
82	Experimental and theoretical study of S 2p and C 1s generalized oscillator strengths in CS2. Journal of Electron Spectroscopy and Related Phenomena, 2007, 155, 21-27.	1.7	3
83	Characterization by27Al NMR, X-ray Absorption Spectroscopy, and Density Functional Theory Techniques of the Species Responsible for Benzene Hydrogenation in Y Zeolite-Supported Carburized Molybdenum Catalysts. Journal of Physical Chemistry B, 2006, 110, 15803-15811.	2.6	12
84	Double ionization of atoms by ion impact: two-step models. Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, 1751-1761.	1.5	16
85	Theoretical investigations on the vibronic coupling between the electronic states S0 and S1 of formic acid including the photodissociation at 248nm. Chemical Physics Letters, 2005, 407, 166-170.	2.6	10
86	Theoretical investigations on valence vibronic transitions. Brazilian Journal of Physics, 2005, 35, 971-980.	1.4	11
87	Young-type interference pattern in molecular inner-shell excitations by electron impact. Physical Review A, 2005, 72, .	2.5	7
88	On the Conformational Memory in the Photodissociation of Formic Acid. Journal of Physical Chemistry A, 2005, 109, 2836-2839.	2.5	18
89	Collisional electron detachment of atomic anions by noble gases: universal behavior at intermediate velocities. Brazilian Journal of Physics, 2004, 34, 825-828.	1.4	3
90	Absolute electron detachment cross sections of atomic anions of the second and third periods incident on noble gases. Physical Review A, 2004, 69, .	2.5	19

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91	Generalized oscillator strength for core excitations of nitrous oxide. Chemical Physics, 2004, 299, 83-88.	1.9	9
92	Forbidden transitions in benzene. Computational and Theoretical Chemistry, 2003, 621, 99-105.	1.5	19
93	Mixed-oxide formation during preparation of alumina-supported zirconia: an EXAFS and DFT study. Physical Chemistry Chemical Physics, 2003, 5, 3811-3817.	2.8	20
94	Laser interaction with a pair of two-dimensional coupled quantum dots. Journal of Applied Physics, 2003, 94, 2579-2584.	2.5	8
95	Contributions to the generalized oscillator strength for the inner-shell C1sâ†'3sÏƒgtransition inCO2from the vibronic coupling mechanism. Physical Review A, 2002, 66, .	2.5	8
96	Direct Investigation of the Validity of Vertical Approximation in the Calculation of Transition Moment Matrix Elements:â€‰ n â†' Ï€* Transition in Methyl Formate. Journal of Physical Chemistry A, 2002, 106, 181-183.	2.5	18
97	Generalized oscillator strengths for C 1s excitation of acetylene and ethylene. Journal of Electron Spectroscopy and Related Phenomena, 2002, 123, 303-314.	1.7	17
98	Generalized oscillator strength profiles for inner shell excitation of CO2 derived from variable angle electron energy loss spectroscopy. Journal of Electron Spectroscopy and Related Phenomena, 2001, 114-116, 93-97.	1.7	9
99	Intensity of the â†' symmetry-forbidden electronic transition in acetone by direct vibronic coupling mechanism. Chemical Physics Letters, 2001, 337, 331-334.	2.6	15
100	Isotopic effects in inner-shell spectrum of methane: a theoretical study. Computational and Theoretical Chemistry, 2001, 539, 145-148.	1.5	8
101	Vibronic coupling for H2CO and CO2. Chemical Physics, 2000, 253, 51-57.	1.9	24
102	Explicit core-hole localization and relaxation effects in the calculation of inner-shell spectrum of C2H4. Journal of Chemical Physics, 2000, 113, 7971-7975.	3.0	8
103	Experimental and theoretical study of generalized oscillator strengths for C1sand O1sexcitations inCO2. Physical Review A, 2000, 61, .	2.5	30
104	Inner-shell excitations of water molecule. Chemical Physics, 1999, 243, 9-15.	1.9	10
105	Optical and generalized oscillator strengths for theB1Î£+,C1Î£+, andE1Îvibronic bands in the CO molecule. Physical Review A, 1998, 57, 4394-4400.	2.5	25
106	Fano-Feshbach Formalism Applied to the Calculation of Autoionization Widths through Analytic Continuation. Journal of Chemical Physics, 0, , .	3.0	0