Itamar Borges

List of Publications by Year
in descending order

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78 papers	1,119 citations	430874 18 h-index	526287 27 g-index
78 all docs	78 docs citations	78 times ranked	1104 citing authors

#	Article	IF	Citations
1	Ab Initio Modeling of Excitonic and Charge-Transfer States in Organic Semiconductors: The PTB1/PCBM Low Band Gap System. Journal of the American Chemical Society, 2013, 135, 18252-18255.	13.7	59
2	Topological Analysis of the Molecular Charge Density and Impact Sensitivy Models of Energetic Molecules. Journal of Physical Chemistry A, 2011, 115, 9055-9068.	2.5	58
3	Brazilian symposium of theoretical chemistry (SBQT2013). Journal of Molecular Modeling, 2015, 21, 1.	1.8	57
4	Density-Functional Theory Simulation of the Dissociative Chemisorption of Water Molecules on the MgO(001) Surface. Journal of Physical Chemistry C, 2012, 116, 738-744.	3.1	45
5	Intermolecular interactions and charge transfer transitions in aromatic hydrocarbonâ€“tetracyanoethylene complexes. Physical Chemistry Chemical Physics, 2014, 16, 20586-20597.	2.8	43
6	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
7	Theoretical Study of the Reaction between HF Molecules and Hydroxyl Layers of Mg(OH)₂. Journal of Physical Chemistry A, 2009, 113, 6494-6499.	2.5	34
8	Density functional theory molecular simulation of thiophene adsorption on MoS2 including microwave effects. Computational and Theoretical Chemistry, 2007, 822, 80-88.	1.5	32
9	Sarin Degradation Using Brucite. Journal of Physical Chemistry C, 2011, 115, 24937-24944.	3.1	30
10	The electronically excited states of RDX (hexahydroâ€1,3,5â€trinitroâ€1,3,5â€triazine): Vertical excitations. International Journal of Quantum Chemistry, 2009, 109, 2348-2355.	2.0	27
11	Optical and generalized oscillator strengths for theB1Î£+,C1Î£+, andE1Îvibronic bands in the CO molecule. Physical Review A, 1998, 57, 4394-4400.	2.5	25
12	Dynamics of benzene excimer formation from the parallel-displaced dimer. Physical Chemistry Chemical Physics, 2019, 21, 13916-13924.	2.8	23
13	Absorption and Fluorescence Spectra of Poly(p-phenylenevinylene) (PPV) Oligomers: An ab Initio Simulation. Journal of Physical Chemistry A, 2015, 119, 1787-1795.	2.5	22
14	Insight into the Excited State Electronic and Structural Properties of the Organic Photovoltaic Donor Polymer Poly(thieno[3,4-b]thiophene benzodithiophene) by Means of ab Initio and Density Functional Theory. Journal of Physical Chemistry C, 2016, 120, 21818-21826.	3.1	22
15	Defesa quÃmica: histÃ³rico, classificaÃ§Ã£o dos agentes de guerra e aÃ§Ã£o dos neurotÃ³xicos. Quimica Nova, 2012, 35, 2083-2091.	0.3	21
16	Potential Energy Curves for X1Î£+ and A1Î States of CO: The A1Î(vâ€²=1â€“23)â†X1Î£+(vâ€³=0, 1) Transitions. Journal of Molecular Spectroscopy, 2001, 209, 24-29.	1.2	20
17	Doubly excited states of molecular hydrogen: theoretical absorption and photodissociation cross sections. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, 1713-1724.	1.5	19
18	Forbidden transitions in benzene. Computational and Theoretical Chemistry, 2003, 621, 99-105.	1.5	19

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19	On the Conformational Memory in the Photodissociation of Formic Acid. Journal of Physical Chemistry A, 2005, 109, 2836-2839.	2.5	18
20	Chemical dynamics simulations of CID of peptide ions: comparisons between TIK(H⁺)₂and TLK(H⁺)₂fragmentation dynamics, and with thermal simulations. Physical Chemistry Chemical Physics, 2018, 20, 3614-3629.	2.8	18
21	Correlation between molecular charge densities and sensitivity of nitrogen-rich heterocyclic nitroazole derivative explosives. Journal of Molecular Modeling, 2019, 25, 314.	1.8	18
22	Valence electronic excitation of the SiF4molecule: generalized oscillator strength for the 5t2â†' 6a1transition andab initiocalculation. Journal of Physics B: Atomic, Molecular and Optical Physics, 2001, 34, 1005-1017.	1.5	16
23	Hydrolysis of a VX-like Organophosphorus Compound through Dissociative Chemisorption on the MgO(001) Surface. Journal of Physical Chemistry C, 2013, 117, 20791-20801.	3.1	16
24	Accurate calculation of near-critical heat capacities C P and C V of argon using molecular dynamics. Journal of Molecular Liquids, 2017, 237, 65-70.	4.9	16
25	On the molecular origin of the sensitivity to impact of cyclic nitramines. International Journal of Quantum Chemistry, 2019, 119, e25868.	2.0	16
26	On the semiclassical dissociation yields of the doubly excited states of H2. Chemical Physics Letters, 2001, 342, 411-416.	2.6	15
27	DFT conformational studies of the HI-6 molecule. International Journal of Quantum Chemistry, 2005, 105, 260-269.	2.0	15
28	Excited electronic and ionized states of the nitramide molecule, H2NNO2, studied by the symmetry-adapted-cluster configuration interaction method. Theoretical Chemistry Accounts, 2008, 121, 239-246.	1.4	15
29	Conformations and charge distributions of diazocyclopropanes. International Journal of Quantum Chemistry, 2008, 108, 2615-2622.	2.0	15
30	Excited electronic and ionized states of N,N-dimethylnitramine. Chemical Physics, 2008, 349, 256-262.	1.9	15
31	Nuclear fukui functions and the deformed atoms in molecules representation of the electron density: Application to gasâ€Phase RDX (hexahydroâ€1,3,5â€trinitroâ€1,3,5â€triazine) electronic structure and decomposition. International Journal of Quantum Chemistry, 2011, 111, 1444-1452.	2.0	14
32	Non-Franck-Condon electron-impact dissociative-excitation cross sections of molecular hydrogen producingH(1s)+H(2l)throughX1Î£g+(v=0)â†'{B1Î£u+,Bâ€²1Î£u+,C1Îu}. Physical Review A, 1998, 57, 1025-1032.	2.5	13
33	Photon and high-energyâ€“electron-impact vibronic excitation of molecular hydrogen. Physical Review A, 1999, 60, 1226-1234.	2.5	13
34	Probing topological electronic effects in catalysis: thiophene adsorption on NiMoS and CoMoS clusters. Journal of the Brazilian Chemical Society, 2012, 23, 1789-1799.	0.6	13
35	Destruction cross sections for fast hydrogen molecules incident on helium, neon, and argon. Physical Review A, 1995, 51, 3831-3836.	2.5	12
36	How to find an optimum cluster size through topological site properties: MoS_xmodel clusters. Journal of Computational Chemistry, 2011, 32, 2186-2194.	3.3	12

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37	Theoretical investigations on valence vibronic transitions. Brazilian Journal of Physics, 2005, 35, 971-980.	1.4	11
38	Configuration interaction oscillator strengths of the H2O molecule: Transitions from the ground to the <mml:math altimg="si13.gif" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.el. Chemical Physics	1.9	11
39	Molecular dynamics simulations of momentum and thermal diffusion properties of near-critical argon along isobars. Journal of Supercritical Fluids, 2016, 114, 46-54.	3.2	11
40	Proton Migration on Perfect, Vacant, and Doped MgO(001) Surfaces: Role of Dissociation Residual Groups. Journal of Physical Chemistry C, 2018, 122, 21841-21853.	3.1	11
41	Electronic and spectroscopic properties of A-series nerve agents. Computational and Theoretical Chemistry, 2021, 1202, 113321.	2.5	11
42	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
43	Electronic spectra of nitroethylene. International Journal of Quantum Chemistry, 2012, 112, 1225-1232.	2.0	10
44	Water solvent effects using continuum and discrete models: The nitromethane molecule, CH₃NO₂. Journal of Computational Chemistry, 2015, 36, 2260-2269.	3.3	10
45	Discrete and continuum modeling of solvent effects in a twisted intramolecular charge transfer system: The 4-N,N-dimethylaminobenzonitrile (DMABN) molecule. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 201, 73-81.	3.9	10
46	Theoretical NMR and conformational analysis of solvated oximes for organophosphates-inhibited acetylcholinesterase reactivation. Journal of Molecular Structure, 2018, 1152, 311-320.	3.6	10
47	Molecular dynamics simulation of the electron ionization mass spectrum of tabun. Journal of Mass Spectrometry, 2020, 55, e4513.	1.6	10
48	Correlation Between Molecular Charge Properties and Impact Sensitivity of Explosives: Nitrobenzene Derivatives. Propellants, Explosives, Pyrotechnics, 2021, 46, 309-321.	1.6	10
49	Formation reaction mechanisms of hydroxide anions from Mg(OH)2 layers. Chemical Physics, 2013, 418, 1-7.	1.9	9
50	Microwave effects on NiMoS and CoMoS single-sheet catalysts. Journal of Molecular Modeling, 2018, 24, 128.	1.8	9
51	Influences on the calculation of accurate and basis set extrapolated oscillator strengths: the transition of H2O. Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, 641-650.	1.5	8
52	Reexamination of the Lyman-Birge-Hopfield transition ofN2: Configuration-interaction generalized oscillator strengths. Physical Review A, 2007, 75, .	2.5	8
53	Electronic and ionization spectra of 1,1-diamino-2,2-dinitroethylene, FOX-7. Journal of Molecular Modeling, 2014, 20, 2095.	1.8	8
54	A Multireference Configuration Interaction Study of the Photodynamics of Nitroethylene. Journal of Physical Chemistry A, 2014, 118, 12011-12020.	2.5	7

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55	The CH3POF2 molecule: ab initio studies of structure, vibrational spectrum and methyl rotational barrier. Computational and Theoretical Chemistry, 2004, 712, 187-195.	1.5	6
56	Accurate non-asymptotic thermodynamic properties of near-critical N2 and O2 computed from molecular dynamics simulations. Journal of Supercritical Fluids, 2018, 135, 225-233.	3.2	6
57	Quantifying bond strengths via a Coulombic force model: application to the impact sensitivity of nitrobenzene, nitrogen-rich nitroazole, and non-aromatic nitramine molecules. Journal of Molecular Modeling, 2021, 27, 69.	1.8	6
58	Photon and electron-impact dissociation cross sections of HCl. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 3703-3711.	1.5	5
59	Rate constants for the CH3Oâ€…+â€…NO â† CH3ONO reaction by classical trajectory and canonical variational transition state theory calculations. Journal of Physical Organic Chemistry, 2002, 15, 123-129.	1.9	5
60	Elucidating the mass spectrum of the retronecine alkaloid using DFT calculations. Journal of Mass Spectrometry, 2018, 53, 934-941.	1.6	5
61	Theoretical analysis of the stabilization of graphene nanosheets by means of strongly polarized pyrene derivatives. Chemical Physics, 2019, 527, 110468.	1.9	5
62	Pronounced changes in atomistic mechanisms for the Cl^{â˜} + CH₃I S_N2 reaction with increasing collision energy. Physical Chemistry Chemical Physics, 2019, 21, 2039-2045.	2.8	5
63	Simulation of the electron ionization mass spectra of the Novichok nerve agent. Journal of Mass Spectrometry, 2021, 56, e4779.	1.6	5
64	Theoretical Chemistry at the Service of the Chemical Defense: Degradation of Nerve Agents in Magnesium Oxide and Hydroxide Surface. Revista Virtual De Quimica, 2014, 6, .	0.4	4
65	Properties of molecular charge distributions affecting the sensitivity of energetic materials. Theoretical and Computational Chemistry, 2022, , 81-105.	0.4	4
66	collisional destruction by He, Ne and Ar. Journal of Physics B: Atomic, Molecular and Optical Physics, 1996, 29, 733-739.	1.5	3
67	Collisional fragmentation of fastHeH+ions: TheHe2++Hâ˜channel. Physical Review A, 1999, 59, 1988-1993.	2.5	3
68	Configuration interaction and relaxation effects on generalized and optical oscillator strengths of the H2O molecule: The X1A1â†'A1B1 transition. Journal of Electron Spectroscopy and Related Phenomena, 2007, 155, 40-46.	1.7	3
69	Molecular Electronic Topology and Fragmentation Onset via Charge Partition Methods and Nuclear Fukui Functions: 1,1-Diamino-2,2-dinitroethylene. Journal of the Brazilian Chemical Society, 2015, , .	0.6	3
70	Adsorption of Trinitrotoluene on a MgO(001) Surface Including Surface Relaxation Effects. Journal of Chemistry, 2013, 2013, 1-8.	1.9	2
71	Electronic structure theory gives insights into the higher efficiency of the PTB electron-donor polymers for organic photovoltaics in comparison with prototypical P3HT. Journal of Chemical Physics, 2018, 149, 184905.	3.0	2
72	COMPARAÃ‡ÃƒO ENTRE MÃ‰TODOS PARA DETERMINAÃ‡ÃƒO DE CARGAS ATÃ”MICAS EM SISTEMAS MOLECULARES: A MOLÃ‰CULA N-{N-(PTERINA-7-IL)CARBONILGLICIL}-L-TIROSINA (NNPT). Quimica Nova, 2020, , .	0.3	2

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73	Nonradiative relaxation mechanisms of the elusive silole molecule. Physical Chemistry Chemical Physics, 2021, 23, 26561-26574.	2.8	2
74	An ab initio study of the structure and methyl rotational barriers of methylphosphonic dihalides. Computational and Theoretical Chemistry, 2005, 718, 105-109.	1.5	1
75	On the interaction of two conical intersections: the H6 system. Chemical Physics Letters, 2000, 331, 285-289.	2.6	0
76	Prioritization of potential agreements between science, technology and innovation institutions: Prospective analysis for sorting countries according to interest areas of Brazilian army from the scientific and technological perspectives. , 2017, , .		0
77	Resenha do Livro "Neither Physics nor Chemistry: a History of Quantum Chemistry". Revista Virtual De Quimica, 2012, 4, .	0.4	0
78	Photoionization Spectra and Ionization Potentials of Energetic Molecules. Progress in Theoretical Chemistry and Physics, 2015, , 147-158.	0.2	0