Francisco B C Machado

List of Publications by Year
in descending order

78	1,524	331670 21	345221 36
papers	citations	h-index	g-index

83	83	83	1802
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Multireference Approaches for Excited States of Molecules. Chemical Reviews, 2018, 118, 7293-7361.	47.7	287
2	The transition metal-carbonyl bond. Accounts of Chemical Research, 1993, 26, 628-635.	15.6	118
3	Ï€â€“Ï€ stacking between polyaromatic hydrocarbon sheets beyond dispersion interactions. Physical Chemistry Chemical Physics, 2016, 18, 22300-22310.	2.8	57
4	A theoretical investigation of the lowâ€lying electronic states of the molecule BeH+. Journal of Chemical Physics, 1991, 94, 7237-7244.	3.0	52
5	Synthesis, characterization, and computational study of a new dimethoxy-chalcone. Journal of Molecular Modeling, 2014, 20, 2526.	1.8	42
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	Radiative transition probabilities and lifetimes for the band systems AÂ²pi - XÂ²sigma+ of the isovalent molecules BeF, MgF and CaF. Brazilian Journal of Physics, 2005, 35, 950-956.	1.4	38
8	A theoretical investigation of some lowâ€lying electronic states of imidazole. Journal of Chemical Physics, 1992, 97, 1881-1891.	3.0	37
9	Theoretical studies of zinc phthalocyanine monomer, dimer and trimer forms. Computational and Theoretical Chemistry, 2009, 899, 71-78.	1.5	35
10	High-level theoretical benchmark investigations of the UV-vis absorption spectra of paradigmatic polycyclic aromatic hydrocarbons as models for graphene quantum dots. Journal of Chemical Physics, 2019, 150, 124302.	3.0	35
11	Excited states and excitonic interactions in prototypic polycyclic aromatic hydrocarbon dimers as models for graphitic interactions in carbon dots. Physical Chemistry Chemical Physics, 2019, 21, 9077-9088.	2.8	34
12	Geometries, Binding Energies, Ionization Potentials, and Electron Affinities of Metal Clusters: Mg_n^{0,ÂÂ±Â1}, n = 1â€“7. Journal of Physical Chemistry C, 2016, 120, 13275-13286.	3.1	32
13	On the lowâ€lying electronic states of the molecule BeN. Journal of Chemical Physics, 1991, 95, 9086-9093.	3.0	30
14	Singlet L_a and L_b Bands for N-Acenes (N = 2â€“7): A CASSCF/CASPT2 Study. Journal of Chemical Theory and Computation, 2017, 13, 4297-4306.	5.3	30
15	Energetic and structural features of the CH4+O(3P)â†’CH3+OH abstraction reaction: Does perturbation theory from a multiconfiguration reference state (finally) provide a balanced treatment of transition states?. Journal of Chemical Physics, 1999, 111, 10046-10052.	3.0	29
16	What is so mysterious about the electronic states of SCI?. Molecular Physics, 2002, 100, 699-704.	1.7	29
17	Metalâ€“Halogen Bonding Seen through the Eyes of Vibrational Spectroscopy. Materials, 2020, 13, 55.	2.9	26
18	Binding energy of chromium hexacarbonyl. 2. Revisited with correlation effects. The Journal of Physical Chemistry, 1993, 97, 4397-4403.	2.9	24

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19	A high level theoretical investigation of the N2O4â†'2â€‰NO2 dissociation reaction: Is there a transition state?. Journal of Chemical Physics, 2003, 118, 4060-4065.	3.0	23
20	A product branching ratio controlled by vibrational adiabaticity and variational effects: Kinetics of the H + trans-N2H2 reactions. Journal of Chemical Physics, 2012, 136, 184310.	3.0	23
21	How to efficiently tune the biradicaloid nature of acenes by chemical doping with boron and nitrogen. Physical Chemistry Chemical Physics, 2017, 19, 19225-19233.	2.8	23
22	A theoretical study of the infrared transition matrix elements for the Xâ€‰1Î£+ state of the CH+ and CD+ molecules. Journal of Chemical Physics, 1986, 84, 1296-1301.	3.0	22
23	Momentum distributions, spin distributions, and bonding in methylamine and its radical cation. Journal of the American Chemical Society, 1992, 114, 6496-6504.	13.7	22
24	A systematic analysis of excitonic properties to seek optimal singlet fission: the BN-substitution patterns in tetracene. Journal of Materials Chemistry C, 2020, 8, 7793-7804.	5.5	22
25	DFT study for the reactions of H atoms with CH₃OH and C₂H₅OH. International Journal of Quantum Chemistry, 2008, 108, 2476-2485.	2.0	18
26	Emission Energies and Stokes Shifts for Single Polycyclic Aromatic Hydrocarbon Sheets in Comparison to the Effect of Excimer Formation. Journal of Physical Chemistry Letters, 2019, 10, 5592-5597.	4.6	18
27	On electron correlation in NaCl2. International Journal of Quantum Chemistry, 1995, 54, 299-304.	2.0	17
28	The electronic states of a double carbon vacancy defect in pyrene: a model study for graphene. Physical Chemistry Chemical Physics, 2015, 17, 12778-12785.	2.8	17
29	Accurate rovibrational energies of ozone isotopologues up to J = 10 utilizing artificial neural networks. Journal of Chemical Physics, 2018, 149, 024307.	3.0	17
30	Pushing 3câ€“4e Bonds to the Limit: A Coupled Cluster Study of Stepwise Fluorination of First-Row Atoms. Inorganic Chemistry, 2019, 58, 14777-14789.	4.0	16
31	N2 activation by iron-sulfur complexes. Theoretica Chimica Acta, 1995, 92, 315-326.	0.8	15
32	Theoretical study on electronâ€“free-radical scattering: An application to CF. Physical Review A, 2002, 66, .	2.5	14
33	MRCI study of the photoelectron spectrum of GeC and GeSi and their GeC+ and GeSi+ ions. International Journal of Quantum Chemistry, 2006, 106, 2677-2688.	2.0	13
34	Hydrogen Abstraction from the Hydrazine Molecule by an Oxygen Atom. Journal of Physical Chemistry A, 2015, 119, 1628-1635.	2.5	12
35	Ruthenium-cymene containing pyridine-derived aldiimine ligands: Synthesis, characterization and application in the transfer hydrogenation of aryl ketones and kinetics studies. Journal of Organometallic Chemistry, 2019, 892, 51-65.	1.8	12
36	Dual-level direct dynamics calculations of deuterium kinetic isotope effects for the Cl(2P)+C2H6 abstraction reaction. Theoretical Chemistry Accounts, 2001, 107, 15-21.	1.4	11

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37	MRSDCI study of the two lower-lying doublet electronic states of the BeB, MgB, and CaB molecules. International Journal of Quantum Chemistry, 2003, 95, 205-212.	2.0	11
38	Direct Dynamics Simulation of the Thermal 3CH2 + 3O2 Reaction. Rate Constant and Product Branching Ratios. Journal of Physical Chemistry A, 2018, 122, 4808-4818.	2.5	11
39	Tuning the Biradicaloid Nature of Polycyclic Aromatic Hydrocarbons: The Effect of Graphitic Nitrogen Doping in Zethrenes. ChemPhysChem, 2018, 19, 2492-2499.	2.1	11
40	A theoretical description of the ionic species BeF2+. Journal of Physics B: Atomic, Molecular and Optical Physics, 1993, 26, 1993-2003.	1.5	10
41	The Diverse Manifold of Electronic States Generated by a Single Carbon Defect in a Graphene Sheet: Multireference Calculations Using a Pyrene Defect Model. ChemPhysChem, 2014, 15, 3334-3341.	2.1	10
42	THE H₂Â+ÂCOÂ ÂH₂CO REACTION: RATE CONSTANTS AND RELEVANCE TO HOT AND DENSE ASTROPHYSICAL MEDIA. Astrophysical Journal, Supplement Series, 2016, 225, 2.	7.7	10
43	Thermochemical and Kinetics of CH₃SH + H Reactions: The Sensitivity of Coupling the Low and High-Level Methodologies. Journal of Physical Chemistry A, 2017, 121, 419-428.	2.5	10
44	Investigation of the ozone formation reaction pathway: Comparisons of full configuration interaction quantum Monte Carlo and fixed-node diffusion Monte Carlo with contracted and uncontracted MRCI. Journal of Chemical Physics, 2017, 147, 094306.	3.0	10
45	The characterization of electronic defect states of single and double carbon vacancies in graphene sheets using molecular density functional theory. Molecular Physics, 2019, 117, 1519-1531.	1.7	10
46	Comparative study of small boron, silicon and germanium clusters: BmSin and BmGen (m + nâ€‰=â€‰2â€“4). Journal of Molecular Modeling, 2015, 21, 141.	1.8	8
47	Electronic structure of CuX^y (X = B, C, N, O, F; y = 0, +1, â^'1). International Journal of Quantum Chemistry, 2008, 108, 2512-2522.	2.0	7
48	A theoretical study of the inversion and rotation barriers in Methyl-substituted Amines. Journal of the Brazilian Chemical Society, 2011, 22, 968-975.	0.6	7
49	A quantitative tool to establish magic number clusters, Îµ3, applied in small silicon clusters, Si2-11. Journal of Molecular Modeling, 2018, 24, 203.	1.8	7
50	Thermochemical and Kinetics of Hydrazine Dehydrogenation by an Oxygen Atom in Hydrazine-Rich Systems: A Dimer Model. Journal of Physical Chemistry A, 2015, 119, 12607-12614.	2.5	7
51	Alkali-metal dihalide molecules: electronic spectrum. The Journal of Physical Chemistry, 1993, 97, 5882-5885.	2.9	6
52	Investigation of strain relaxation mechanism in small SiGe clusters. Physica Status Solidi (B): Basic Research, 2007, 244, 3601-3611.	1.5	6
53	Theoretical study of the Ge_mSi_n (m + n = 3) clusters. International Journal of Quantum Chemistry, 2011, 111, 1562-1569.	2.0	6
54	Hydrazine decomposition on a small platinum cluster: the role of N2H5 intermediate. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	6

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55	Interplay between Aromaticity and Radicaloid Character in Nitrogen-Doped Oligoacenes Revealed by High-Level Multireference Methods. Journal of Physical Chemistry A, 2018, 122, 9464-9473.	2.5	6
56	A Proposal for the Mechanism of the CH + CO2 Reaction. ACS Omega, 2019, 4, 17843-17849.	3.5	5
57	Potential Energy Curves for Formation of the CH2O2 Criegee Intermediate on the 3CH2 + 3O2 Singlet and Triplet Potential Energy Surfaces. Journal of Physical Chemistry A, 2019, 123, 8968-8975.	2.5	5
58	Effects on the aromaticity and on the biradicaloid nature of acenes by the inclusion of a cyclobutadiene linkage. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	5
59	Multireference study of ionic/covalent electronic states of MF (MÂ=ÂBe, Mg and Ca). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 233, 118210.	3.9	5
60	Relating Bond Strength and Nature to the Thermodynamic Stability of Hypervalent Togniâ€Type Iodine Compounds. ChemPlusChem, 2021, 86, 1199-1210.	2.8	5
61	The influence of the environment in chemical reactivity: the HCOOH formation from the H2O + CO reaction. Journal of Molecular Modeling, 2021, 27, 264.	1.8	5
62	Theoretical calculations of structures, energetics, and kinetics of O (³P) + CH₃OH reactions. International Journal of Quantum Chemistry, 2010, 110, 2037-2046.	2.0	4
63	Implications of the (H2O)nÂ+ÂCO â†" trans-HCOOHÂ+Â(H2O)nâ€"1 (nÂ=Â1, 2, and 3) reactions for primordial atmospheres of Venus and Earth. Monthly Notices of the Royal Astronomical Society, 2018, 475, 3191-3200.	4.4	4
64	Electronic structure and stability of transition metal acetylacetonates TM(AcAc)n (TMÂ=ÂCr, Fe, Co, Ni,) Tj ETQq0 0 0 rgBT /Overlock 10	2.5	4
65	A multireference configuration interaction study of CuB and CuAl molecular constants and photoionization spectra. Journal of Chemical Physics, 2013, 139, 124316.	3.0	3
66	Thermochemical and kinetics studies of the CH3SH+S (3P) hydrogen abstraction and insertion reactions. Journal of Molecular Modeling, 2014, 20, 2449.	1.8	3
67	On the importance of non-covalent interactions for porous membranes: unraveling the role of pore size. Physical Chemistry Chemical Physics, 2018, 20, 20124-20131.	2.8	3
68	Could HCN Be Responsible for the Formamide Synthesis in Earthâ€™s Primitive Atmosphere?. Astrophysical Journal, Supplement Series, 2019, 245, 11.	7.7	3
69	Accurate Rate Constants for the Forward and Reverse H + CO â†" HCO Reactions at the High-Pressure Limit. ACS Omega, 2020, 5, 23975-23982.	3.5	3
70	Ab initio calculations on XFnq (X = I, Xe, Cs, and Ba;n=1, 2, 4, and 6;q=?1, 0, +1, and +2) molecules. International Journal of Quantum Chemistry, 2001, 81, 238-245.	2.0	2
71	A CASSCF/MRCI study of the lowâ€lying electronic states of the BeS molecule. International Journal of Quantum Chemistry, 2011, 111, 1694-1700.	2.0	2
72	Thermochemical and Kinetics of the CH₃OH + (⁴S)N Reactional System. Journal of Physical Chemistry A, 2018, 122, 5905-5910.	2.5	2

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73	Stability and Reactivity of Silicon Magic Numbers Doped with Aluminum and Phosphorus Atoms. Journal of Physical Chemistry A, 2019, 123, 247-256.	2.5	2
74	Identification of Magic Numbers in Homonuclear Clusters: The Îµ³ Stability Ranking Function. Journal of Physical Chemistry A, 2020, 124, 454-463.	2.5	2
75	Methanol and glycolaldehyde production from formaldehyde in massive star-forming regions. Monthly Notices of the Royal Astronomical Society, 2020, 497, 4486-4494.	4.4	2
76	Tunneling Enhancement of the Gas-Phase CH + CO₂ Reaction at Low Temperature. Journal of Physical Chemistry A, 2020, 124, 10717-10725.	2.5	1
77	The relativistic effects on the methane activation by gold(I) cations. Journal of Chemical Physics, 2021, 154, 244113.	3.0	1
78	Reply to â€œComment on â€˜Thermochemical and Kinetics of the CH3OH+(4S)N Reactional Systemâ€™â€• Journal of Physical Chemistry A, 2019, 123, 967-969.	2.5	0