# 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 | Electronic structure and stability of transition metal acetylacetonates TM(AcAc)n (TMÂ=ÂCr, Fe, Co, Ni,) Tj ETQq1 1 0.784314 rgBT /Ove | 2.5 | 4 |
| 2 | The relativistic effects on the methane activation by gold(I) cations. Journal of Chemical Physics, 2021, 154, 244113. | 3.0 | 1 |
| 3 | Relating Bond Strength and Nature to the Thermodynamic Stability of Hypervalent Togniâ€Type Iodine Compounds. ChemPlusChem, 2021, 86, 1199-1210. | 2.8 | 5 |
| 4 | 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 |
| 5 | Identification of Magic Numbers in Homonuclear Clusters: The Îµ<sup>3</sup> Stability Ranking Function. Journal of Physical Chemistry A, 2020, 124, 454-463. | 2.5 | 2 |
| 6 | Metalâ€“Halogen Bonding Seen through the Eyes of Vibrational Spectroscopy. Materials, 2020, 13, 55. | 2.9 | 26 |
| 7 | 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 |
| 8 | Tunneling Enhancement of the Gas-Phase CH + CO<sub>2</sub> Reaction at Low Temperature. Journal of Physical Chemistry A, 2020, 124, 10717-10725. | 2.5 | 1 |
| 9 | 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 |
| 10 | 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 |
| 11 | The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110. | 3.0 | 42 |
| 12 | 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 |
| 13 | 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 |
| 14 | 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 |
| 15 | A Proposal for the Mechanism of the CH + CO2 Reaction. ACS Omega, 2019, 4, 17843-17849. | 3.5 | 5 |
| 16 | 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 |
| 17 | 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 |
| 18 | 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 |

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|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | 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 |
| 22 | Could HCN Be Responsible for the Formamide Synthesis in Earthâ€™s Primitive Atmosphere?. Astrophysical Journal, Supplement Series, 2019, 245, 11. | 7.7 | 3 |
| 23 | 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 |
| 24 | 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 |
| 25 | 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 |
| 26 | 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 |
| 27 | 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 |
| 28 | Thermochemical and Kinetics of the CH<sub>3</sub>OH + (<sup>4</sup>S)N Reactional System. Journal of Physical Chemistry A, 2018, 122, 5905-5910. | 2.5 | 2 |
| 29 | Multireference Approaches for Excited States of Molecules. Chemical Reviews, 2018, 118, 7293-7361. | 47.7 | 287 |
| 30 | Tuning the Biradicaloid Nature of Polycyclic Aromatic Hydrocarbons: The Effect of Graphitic Nitrogen Doping in Zethrenes. ChemPhysChem, 2018, 19, 2492-2499. | 2.1 | 11 |
| 31 | Accurate rovibrational energies of ozone isotopologues up to J = 10 utilizing artificial neural networks. Journal of Chemical Physics, 2018, 149, 024307. | 3.0 | 17 |
| 32 | 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 |
| 33 | 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 |
| 34 | Thermochemical and Kinetics of CH<sub>3</sub>SH + H Reactions: The Sensitivity of Coupling the Low and High-Level Methodologies. Journal of Physical Chemistry A, 2017, 121, 419-428. | 2.5 | 10 |
| 35 | 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 |
| 36 | Singlet L<sub>a</sub> and L<sub>b</sub> Bands for N-Acenes (N = 2â€“7): A CASSCF/CASPT2 Study. Journal of Chemical Theory and Computation, 2017, 13, 4297-4306. | 5.3 | 30 |

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|---|---|---|---|
| 37 | 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 |
| 38 | THE H<sub>2</sub>Â+ÂCOÂ ÂH<sub>2</sub>CO REACTION: RATE CONSTANTS AND RELEVANCE TO HOT AND DENSE ASTROPHYSICAL MEDIA. Astrophysical Journal, Supplement Series, 2016, 225, 2. | 7.7 | 10 |
| 39 | Ï€â€“Ï€ stacking between polyaromatic hydrocarbon sheets beyond dispersion interactions. Physical Chemistry Chemical Physics, 2016, 18, 22300-22310. | 2.8 | 57 |
| 40 | Geometries, Binding Energies, Ionization Potentials, and Electron Affinities of Metal Clusters: Mg<sub>n</sub><sup>0,ÂÂ±Â1</sup>, n = 1â€“7. Journal of Physical Chemistry C, 2016, 120, 13275-13286. | 3.1 | 32 |
| 41 | Hydrazine decomposition on a small platinum cluster: the role of N2H5 intermediate. Theoretical Chemistry Accounts, 2016, 135, 1. | 1.4 | 6 |
| 42 | 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 |
| 43 | 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 |
| 44 | Hydrogen Abstraction from the Hydrazine Molecule by an Oxygen Atom. Journal of Physical Chemistry A, 2015, 119, 1628-1635. | 2.5 | 12 |
| 45 | 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 |
| 46 | Synthesis, characterization, and computational study of a new dimethoxy-chalcone. Journal of Molecular Modeling, 2014, 20, 2526. | 1.8 | 42 |
| 47 | 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 |
| 48 | Thermochemical and kinetics studies of the CH3SH+S (3P) hydrogen abstraction and insertion reactions. Journal of Molecular Modeling, 2014, 20, 2449. | 1.8 | 3 |
| 49 | A multireference configuration interaction study of CuB and CuAl molecular constants and photoionization spectra. Journal of Chemical Physics, 2013, 139, 124316. | 3.0 | 3 |
| 50 | 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 |
| 51 | 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 |
| 52 | Theoretical study of the Ge<sub>m</sub>Si<sub>n</sub> (m + n = 3) clusters. International Journal of Quantum Chemistry, 2011, 111, 1562-1569. | 2.0 | 6 |
| 53 | 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 |
| 54 | Theoretical calculations of structures, energetics, and kinetics of O (<sup>3</sup>P) + CH<sub>3</sub>OH reactions. International Journal of Quantum Chemistry, 2010, 110, 2037-2046. | 2.0 | 4 |

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|---|---|---|---|
| 55 | Theoretical studies of zinc phthalocyanine monomer, dimer and trimer forms. Computational and Theoretical Chemistry, 2009, 899, 71-78. | 1.5 | 35 |
| 56 | DFT study for the reactions of H atoms with CH<sub>3</sub>OH and C<sub>2</sub>H<sub>5</sub>OH. International Journal of Quantum Chemistry, 2008, 108, 2476-2485. | 2.0 | 18 |
| 57 | Electronic structure of CuX<sup>y</sup> (X = B, C, N, O, F; y = 0, +1, â^'1). International Journal of Quantum Chemistry, 2008, 108, 2512-2522. | 2.0 | 7 |
| 58 | Investigation of strain relaxation mechanism in small SiGe clusters. Physica Status Solidi (B): Basic Research, 2007, 244, 3601-3611. | 1.5 | 6 |
| 59 | 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 |
| 60 | 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 |
| 61 | 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 |
| 62 | 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 |
| 63 | Theoretical study on electronâ€“free-radical scattering: An application to CF. Physical Review A, 2002, 66, . | 2.5 | 14 |
| 64 | What is so mysterious about the electronic states of SCl?. Molecular Physics, 2002, 100, 699-704. | 1.7 | 29 |
| 65 | 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 |
| 66 | 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 |
| 67 | 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 |
| 68 | On electron correlation in NaCl2. International Journal of Quantum Chemistry, 1995, 54, 299-304. | 2.0 | 17 |
| 69 | N2 activation by iron-sulfur complexes. Theoretica Chimica Acta, 1995, 92, 315-326. | 0.8 | 15 |
| 70 | The transition metal-carbonyl bond. Accounts of Chemical Research, 1993, 26, 628-635. | 15.6 | 118 |
| 71 | Binding energy of chromium hexacarbonyl. 2. Revisited with correlation effects. The Journal of Physical Chemistry, 1993, 97, 4397-4403. | 2.9 | 24 |
| 72 | Alkali-metal dihalide molecules: electronic spectrum. The Journal of Physical Chemistry, 1993, 97, 5882-5885. | 2.9 | 6 |

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| 73 | A theoretical description of the ionic species BeF2+. Journal of Physics B: Atomic, Molecular and Optical Physics, 1993, 26, 1993-2003. | 1.5 | 10 |
| 74 | A theoretical investigation of some lowâ€lying electronic states of imidazole. Journal of Chemical Physics, 1992, 97, 1881-1891. | 3.0 | 37 |
| 75 | 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 |
| 76 | A theoretical investigation of the lowâ€lying electronic states of the molecule BeH+. Journal of Chemical Physics, 1991, 94, 7237-7244. | 3.0 | 52 |
| 77 | On the lowâ€lying electronic states of the molecule BeN. Journal of Chemical Physics, 1991, 95, 9086-9093. | 3.0 | 30 |
| 78 | 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 |