Breno GalvÃ£o

List of Publications by Year
in descending order

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51	512	759233	794594
papers	citations	12 h-index	19 g-index

52	52	52	386
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Accurate Double Many-Body Expansion Potential Energy Surface for N₃(⁴Aâ€²â€²) from Correlation Scaled ab Initio Energies with Extrapolation to the Complete Basis Set Limit. Journal of Physical Chemistry A, 2009, 113, 14424-14430.	2.5	51
2	Emerging contaminants removal by granular activated carbon obtained from residual Macauba biomass. Environmental Science and Pollution Research, 2018, 25, 26482-26492.	5.3	36
3	Quasiclassical Trajectory Study of Atom-Exchange and Vibrational Relaxation Processes in Collisions of Atomic and Molecular Nitrogen. Journal of Physical Chemistry A, 2010, 114, 6063-6070.	2.5	28
4	N(4Sâ€‰/2D)+N2: Accurate ab initio-based DMBE potential energy surfaces and surface-hopping dynamics. Journal of Chemical Physics, 2012, 137, 22A515.	3.0	27
5	Ab Initio Based Double-Sheeted DMBE Potential Energy Surface for N₃(²Aâ€³) and Exploratory Dynamics Calculations. Journal of Physical Chemistry A, 2011, 115, 12390-12398.	2.5	26
6	Electronic Quenching of N(²D) by N₂: Theoretical Predictions, Comparison with Experimental Rate Constants, and Impact on Atmospheric Modeling. Journal of Physical Chemistry Letters, 2013, 4, 2292-2297.	4.6	22
7	Electronic Quenching in N(²D) + N₂ Collisions: A State-Specific Analysis via Surface Hopping Dynamics. Journal of Chemical Theory and Computation, 2014, 10, 1872-1877.	5.3	16
8	Modeling Cusps in Adiabatic Potential Energy Surfaces. Journal of Physical Chemistry A, 2015, 119, 1415-1421.	2.5	15
9	Exploring the MP2 energy surface of nanoalloy clusters with a genetic algorithm: Application to sodiumâ€“potassium. Chemical Physics Letters, 2015, 639, 135-141.	2.6	15
10	What Electronic Structure Method Can Be Used in the Global Optimization of Nanoclusters?. Journal of Physical Chemistry A, 2019, 123, 10454-10462.	2.5	15
11	Reliability of semiempirical and DFTB methods for the global optimization of the structures of nanoclusters. Journal of Molecular Modeling, 2020, 26, 303.	1.8	15
12	Accurate Explicit-Correlation-MRCI-Based DMBE Potential-Energy Surface for Ground-State CNO. Journal of Physical Chemistry A, 2018, 122, 4198-4207.	2.5	13
13	Modeling cusps in adiabatic potential energy surfaces using a generalized Jahn-Teller coordinate. Chemical Physics Letters, 2016, 660, 55-59.	2.6	12
14	Adsorption of CO2 on biphasic and amorphous calcium phosphates: An experimental and theoretical analysis. Chemical Physics Letters, 2019, 714, 143-148.	2.6	12
15	A new active learning approach for global optimization of atomic clusters. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	12
16	Oxidative desulfurization of dibenzothiophene over highly dispersed Mo-doped graphitic carbon nitride. Chemical Papers, 2022, 76, 3401-3412.	2.2	12
17	Energy-switching potential energy surface for the water molecule revisited: A highly accurate singled-sheeted form. Journal of Chemical Physics, 2008, 129, 044302.	3.0	11
18	Theoretical study of small sodiumâ€“potassium alloy clusters through genetic algorithm and quantum chemical calculations. Physical Chemistry Chemical Physics, 2014, 16, 8895-8904.	2.8	11

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19	Structure and stability of neutral Alâ€“Mg nanoclusters up to 55 atoms. Physical Chemistry Chemical Physics, 2016, 18, 31579-31585.	2.8	10
20	Nonadiabatic reaction dynamics to silicon monosulfide (SiS): A key molecular building block to sulfur-rich interstellar grains. Science Advances, 2021, 7, .	10.3	10
21	SiS formation via gas phase reactions between atomic silicon and sulphur-bearing species. Monthly Notices of the Royal Astronomical Society, 2020, 493, 299-304.	4.4	10
22	SiS Formation in the Interstellar Medium through Si+SH Gas-phase Reactions. Astrophysical Journal, 2021, 920, 37.	4.5	10
23	Vibrational energy transfer in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si20.gif" overflow="scroll"><mml:mrow><mml:mi mathvariant="normal">N</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:msup><mml:mrow) Tj ETQq1 1 0.784314 rgBT /Overl	2.6	9
24	mathvariant="normal">N</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:s A genetic algorithm survey on closed-shell atomic nitrogen clusters employing a quantum chemical approach. Journal of Molecular Modeling, 2018, 24, 196.	1.8	9
25	Structural and homotop optimization of neutral Alâ€“Si nanoclusters. Physical Chemistry Chemical Physics, 2018, 20, 17464-17470.	2.8	9
26	Accurate Study of the Two Lowest Singlet States of HN₃: Stationary Structures and Energetics at the MRCI Complete Basis Set Limit. Journal of Physical Chemistry A, 2013, 117, 4044-4050.	2.5	7
27	Quasiclassical Study of the C(³P) + NO(X²Î) and O(³P) + CN(X²Î£⁺) Collisional Processes on an Accurate DMBE Potential Energy Surface. Journal of Physical Chemistry A, 2019, 123, 7195-7200.	2.5	7
28	Dinuclear copper(II) complex with a benzimidazole derivative: Crystal structure, theoretical calculations, and cytotoxic activity. Applied Organometallic Chemistry, 2020, 34, e5425.	3.5	7
29	Exploring the Utility of Many-Body Expansions: A Consistent Set of Accurate Potentials for the Lowest Quartet and Doublet States of the Azide Radical with Revisited Dynamics. Journal of Physical Chemistry A, 2014, 118, 10127-10133.	2.5	6
30	Accurate theoretical predictions on the mechanisms of OSiS formation and its dissociation channels. Monthly Notices of the Royal Astronomical Society, 2018, 481, 1858-1861.	4.4	6
31	A trajectory surface hopping study of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si45.svg"><mml:mrow><mml:msub><mml:mrow><mml:mtext>N</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:m mathvariant="normal">Î£</mml:mi></mml:mrow><mml:mrow><mml:mi>u</mml:mi></mml:mrow><mml:mrow><mml:mo>+</mml:m Chemical Physics Letters, 2019, 729, 61-64.	2.6	6
32	Growth analysis of sodium-potassium alloy clusters from 7 to 55 atoms through a genetic algorithm approach. Journal of Molecular Modeling, 2014, 20, 2421.	1.8	5
33	Accurate Potential Energy Surface for Quartet State HN₂ and Interplay of N(⁴S) + NH(XÌƒ³Î£^{â€“}) versus H + N₂(A³Î£_u⁺) Reactions. Journal of Physical Chemistry A, 2020, 124, 781-789.	2.5	5
34	Chemical dynamics study on the gas-phase reaction of the D1-silylidyne radical (SiD; X²Î) with deuterium sulfide (D₂S) and hydrogen sulfide (H₂S). Physical Chemistry Chemical Physics, 2021, 23, 13647-13661.	2.8	5
35	Gas-Phase Preparation of Silyl Cyanide (SiH₃CN) via a Radical Substitution Mechanism. Journal of the American Chemical Society, 2022, 144, 8649-8657.	13.7	5
36	Theoretical study on the structure and reactions of uranium fluorides. Journal of Molecular Modeling, 2018, 24, 197.	1.8	4

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37	Non-Adiabatic Reaction Dynamics in the Gas-Phase Formation of Phosphinidenesilylene, the Isovalent Counterpart of Hydrogen Isocyanide, under Single-Collision Conditions. Journal of Physical Chemistry Letters, 2021, 12, 2489-2495.	4.6	4
38	Interconversion mechanisms of PN and PO in the interstellar medium through simple atomâ€“diatom collisions. Monthly Notices of the Royal Astronomical Society, 2021, 507, 1899-1903.	4.4	4
39	Stability of neutral molecular polynitrogens: energy content and decomposition mechanisms. RSC Advances, 2021, 11, 21567-21578.	3.6	4
40	Quasiclassical trajectory study of the rotational distribution for the O+NO(v = 0) fundamental vibrational excitation. International Journal of Chemical Kinetics, 2011, 43, 345-352.	1.6	3
41	A method for predicting basins in the global optimization of nanoclusters with applications to AlxCuy alloys. Physical Chemistry Chemical Physics, 2020, 22, 16914-16925.	2.8	3
42	Accurate DMBE potential-energy surface for CNO(2Aâ€³) and rate coefficients in C(3P)+NO collisions. Journal of Chemical Physics, 2021, 154, 034303.	3.0	3
43	The effect of intersystem crossings in N(2D) + H2 collisions. Journal of Chemical Physics, 2015, 142, 184302.	3.0	2
44	Accurate multi-reference study of Si3 electronic manifold. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	2
45	An ab initio investigation of the adsorption properties of water on binary AlSi clusters. Physical Chemistry Chemical Physics, 2020, 22, 24669-24676.	2.8	2
46	Quasiclassical Trajectory Study of the Si + SH Reaction on an Accurate Double Many-Body Expansion Potential Energy Surface. Journal of Physical Chemistry A, 2022, 126, 3555-3568.	2.5	2
47	The SiÂ+ÂSO2 collision and an extended network of neutralâ€“neutral reactions between silicon and sulphur bearing species. Monthly Notices of the Royal Astronomical Society, 2022, 515, 369-377.	4.4	2
48	A Crossed Molecular Beams and Computational Study of the Formation of the Astronomically Elusive Thiosilaformyl Radical (HSiS, X2Aâ€²). Journal of Physical Chemistry Letters, 2021, 12, 5979-5986.	4.6	1
49	Thermochromism in Polydiacetylene/Poly(vinyl alcohol) Hydrogels Obtained by the Freezeâ€“Thaw Method: A Theoretical and Experimental Study. Industrial & Engineering Chemistry Research, 2021, 60, 13243-13252.	3.7	1
50	Mechanisms for N 3 formation in radiated solid nitrogen: Computational predictions including excited electronic states. International Journal of Quantum Chemistry, 2021, 121, e26562.	2.0	0
51	Directed gas-phase preparation of the elusive phosphinosilylidyne (SiPH2, X2Aâ€²â€²) and cis/trans phosphinidenesilyl (HSiPH; X2Aâ€²) radicals under single-collision conditions. Physical Chemistry Chemical Physics, 2021, 23, 18506-18516.	2.8	0