Miguel Paniagua

List of Publications by Year
in descending order

57 papers	1,914 citations	257450 24 h-index	254184 43 g-index
57 all docs	57 docs citations	57 times ranked	558 citing authors

#	Article	IF	Citations
1	Vibrational energy relaxation dynamics of diatomic molecules inside superfluid helium nanodroplets. The case of the I₂molecule. Physical Chemistry Chemical Physics, 2018, 20, 118-130.	2.8	11
2	Dynamics of the O + H2+ â†' OH+ + H, OH + H+ proton and hydrogen atom transfer reactions on the two lowest potential energy surfaces. Physical Chemistry Chemical Physics, 2017, 19, 3857-3868.	2.8	5
3	Potential energy surfaces and quasiclassical trajectory study of the O + H2+â†' OH++ H, OH + H+proton and hydrogen atom transfer reactions and isotopic variants (D2+, HD+). Physical Chemistry Chemical Physics, 2014, 16, 23594-23603.	2.8	25
4	Theoretical approach to the structure, energy and electronic spectroscopy of O@(⁴He)_Ndoped nanodroplets. RSC Advances, 2014, 4, 44972-44979.	3.6	5
5	Full dimensional potential energy surface for the ground state of $mathbf {H_4^+}$H4+ system based on triatomic-in-molecules formalism. Journal of Chemical Physics, 2013, 139, 184302.	3.0	16
6	Basis set convergence of potential energy surfaces: Ground electronic state of H₂ and H. International Journal of Quantum Chemistry, 2011, 111, 387-399.	2.0	12
7	Potential energy surface and reactive collisions for the Au+H2 system. Journal of Chemical Physics, 2010, 132, 034301.	3.0	16
8	The H3+ rovibrational spectrum revisited with a global electronic potential energy surface. Journal of Chemical Physics, 2008, 129, 084307.	3.0	85
9	Transition state spectroscopy of open shell systems: Angle-resolved photodetachment spectra for the adiabatic singlet states of OHF. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 145-160.	3.9	21
10	Coupled diabatic potential energy surfaces for studying the nonadiabatic dynamics at conical intersections in angular resolved photodetachment simulations of OHFâ^'â†'OHF+eâ^'. Journal of Chemical Physics, 2006, 125, 164321.	3.0	31
11	Quantum approaches for the insertion dynamics of the H++D2 and D++H2 reactive collisions. Journal of Chemical Physics, 2005, 123, 194309.	3.0	61
12	F+OH reactive collisions on new excited Aâ€³3 and Aâ€²3 potential-energy surfaces. Journal of Chemical Physics, 2005, 123, 114310.	3.0	44
13	Photodetachment spectrum of OHF[sup â^']: Three-dimensional study of the heavyâ€"lightâ€"heavy resonances. Journal of Chemical Physics, 2004, 121, 309.	3.0	36
14	Transition state dynamics of OHF on several electronic states: Photodetachment spectrum of OHFâ^' and conical intersections. Journal of Chemical Physics, 2004, 121, 9865-9875.	3.0	14
15	Dynamics and kinetics of the F+OH reaction on the ground triplet potential energy surface. Chemical Physics Letters, 2004, 383, 25-30.	2.6	40
16	Quantum stereodynamics of the F+OH(v,â€‰j) reactive collision on the 13Aâ€³ state. Molecular Physics, 2004, 102, 2381-2392.	1.7	22
17	Direct versus resonances mediated F+OH collisions on a new 3Aâ€³ potential energy surface. Journal of Chemical Physics, 2004, 121, 4605-4618.	3.0	45
18	Transition state spectroscopy of the excited electronic states of Liâ€"HF. Journal of Chemical Physics, 2003, 119, 10088-10104.	3.0	35

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19	D3+rovibrational levels and spectra for the adiabatic 11Aâ€² and 13Aâ€² electronic states. Physical Chemistry Chemical Physics, 2002, 4, 6012-6017.	2.8	18
20	Transition state spectroscopy of the excited electronic states of Liî—¸HF. Chemical Physics Letters, 2002, 351, 295-301.	2.6	4
21	Global fit of ab initio potential energy surfaces: II.1. Tetraatomic systems. Computer Physics Communications, 2001, 134, 97-109.	7.5	26
22	Global fit of ab initio potential energy surfaces:ÂII.2. Tetratomic systems A2B2 and ABC2. Computer Physics Communications, 2001, 140, 412-417.	7.5	14
23	Exploring the transition state for the Li+HFâ†'LiF+H reaction through the Aâ†X absorption spectrum and Xâ†A stimulated emission pumping. Journal of Chemical Physics, 2001, 114, 3440-3448.	3.0	14
24	The lowest triplet state 3Aâ€² of H3+: Global potential energy surface and vibrational calculations. Journal of Chemical Physics, 2001, 114, 2182-2191.	3.0	53
25	Global potential energy surfaces for the H3+ system. Analytical representation of the adiabatic ground-state 1â€Š1Aâ€² potential. Journal of Chemical Physics, 2000, 112, 1240-1254.	3.0	107
26	State-to-state reaction probabilities using bond coordinates: Application to the Li+HF(v,â€Šj) collision. Journal of Chemical Physics, 2000, 113, 1781-1794.	3.0	56
27	Global nine-dimensional potential energy surface for the H5 system. I. Ab initio multiple reference single and double excitation configuration interaction computations. Journal of Chemical Physics, 1999, 110, 7789-7795.	3.0	2
28	Global nine-dimensional potential energy surface for the H5 system. II. Fit to an analytical expression. Journal of Chemical Physics, 1999, 110, 7796-7801.	3.0	11
29	Transition state spectroscopy via infrared excitation of Liâ‹¯HF and Liâ‹¯DF van der Waals precursors. Journal of Chemical Physics, 1999, 111, 6712-6723.	3.0	39
30	Global fit of ab initio potential energy surfaces I. Triatomic systems. Computer Physics Communications, 1998, 108, 259-266.	7.5	127
31	Second-order density functional calculations of the MgFH potential energy surface. Computational and Theoretical Chemistry, 1998, 426, 165-169.	1.5	4
32	Quantum stereodynamics of the Li+HF(v,j) reactive collision for different initial states of the reagent. Journal of Chemical Physics, 1998, 109, 9391-9400.	3.0	64
33	Transition state spectroscopy on the Li-HF system. Journal of Chemical Physics, 1998, 109, 2971-2974.	3.0	32
34	Quantum study of the Li+HFâ†'LiF+H reaction. Journal of Chemical Physics, 1997, 107, 10085-10095.	3.0	77
35	Potential energy surface and wave packet calculations on the Li+HFâ†'LiF+H reaction. Journal of Chemical Physics, 1997, 106, 1013-1025.	3.0	65
36	Application of second-order density functional methods to the calculation of the BeFH potential energy surface. International Journal of Quantum Chemistry, 1997, 61, 491-497.	2.0	7

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37	Searching critical points of fitted potential energy surfaces. Computational and Theoretical Chemistry, 1996, 371, 85-90.	1.5	7
38	Potential-energy surfaces for the Li+HF reaction. MRDCI study of the ground- and lower excited-states for doublet LiFH. Chemical Physics, 1995, 201, 107-120.	1.9	44
39	The potential energy surface of the CaHF system. Computational and Theoretical Chemistry, 1995, 341, 123-132.	1.5	3
40	The vibrational structure of H+4 and D+4. Journal of Chemical Physics, 1995, 102, 5725-5732.	3.0	13
41	Accurate global fit of the H4potential energy surface. Journal of Chemical Physics, 1994, 101, 4004-4010.	3.0	75
42	Application of second-order density functional methods to the calculation of the LiFH potential energy surface. International Journal of Quantum Chemistry, 1994, 52, 935-945.	2.0	14
43	Ground- and lowest excited-state MRDCI potential-energy surfaces for the collinear Li+HF reaction. Chemical Physics, 1993, 178, 357-362.	1.9	14
44	Accurate fit of the two lowest excitedâ€state potentialâ€energy surfaces for doublet HeH2+. Journal of Chemical Physics, 1993, 98, 308-315.	3.0	40
45	A new functional form to obtain analytical potentials of triatomic molecules. Journal of Chemical Physics, 1992, 96, 1265-1275.	3.0	308
46	An accurate fit of the potential energy surface of the BeHF system. Computational and Theoretical Chemistry, 1992, 260, 179-193.	1.5	10
47	Scalar and vector properties of the magnesium + hydrogen fluoride reaction on a bond order surface. The Journal of Physical Chemistry, 1991, 95, 8379-8384.	2.9	24
48	Calculation of two-center one-electron molecular integrals with STOs. Computer Physics Communications, 1991, 64, 329-342.	7.5	19
49	Accurate and model collinear reactive probabilities of the Mg+FH reaction. Chemical Physics Letters, 1990, 168, 441-447.	2.6	10
50	Rotation of real spherical harmonics. Computer Physics Communications, 1989, 52, 323-331.	7.5	21
51	Analysis of the electronic correlation energy in the LiFH PES using density functional methods. Chemical Physics, 1989, 134, 287-296.	1.9	17
52	Two-configuration potential energy surface for the Ca + HF â†' CaF + H reaction. Chemical Physics, 1987, 114, 241-249.	1.9	6
53	Two-configuration mc potential energy surface for the reaction of Mg with HF. Chemical Physics, 1986, 101, 55-65.	1.9	14
54	Two-configuration potential energy surface for the collinear Ca + HF â†' CaF + H reaction. Chemical Physics Letters, 1986, 126, 330-334.	2.6	13

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55	Atomic partitioning of two-center potentials for slater basis. International Journal of Quantum Chemistry, 1986, 29, 1155-1164.	2.0	3
56	Relative stability of the2 A 1g and2 E g states of the C2H 6 + ion. Theoretica Chimica Acta, 1979, 53, 377-381.	0.8	8
57	Theoretical study of the ethane ionization spectra within the correlation hole model. Theoretica Chimica Acta, 1979, 54, 53-58.	0.8	7