

Miguel Paniagua

List of Publications by Year in descending order

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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	A new functional form to obtain analytical potentials of triatomic molecules. Journal of Chemical Physics, 1992, 96, 1265-1275.	3.0	308
2	Global fit of ab initio potential energy surfaces I. Triatomic systems. Computer Physics Communications, 1998, 108, 259-266.	7.5	127
3	Global potential energy surfaces for the H ₃ ⁺ system. Analytical representation of the adiabatic ground-state $1\ \hat{A}'\ \hat{e}^2$ potential. Journal of Chemical Physics, 2000, 112, 1240-1254.	3.0	107
4	The H ₃ ⁺ rovibrational spectrum revisited with a global electronic potential energy surface. Journal of Chemical Physics, 2008, 129, 084307.	3.0	85
5	Quantum study of the Li+HF(\hat{v}) \hat{v} 'LiF+H reaction. Journal of Chemical Physics, 1997, 107, 10085-10095.	3.0	77
6	Accurate global fit of the H ₄ potential energy surface. Journal of Chemical Physics, 1994, 101, 4004-4010.	3.0	75
7	Potential energy surface and wave packet calculations on the Li+HF(\hat{v}) \hat{v} 'LiF+H reaction. Journal of Chemical Physics, 1997, 106, 1013-1025.	3.0	65
8	Quantum stereodynamics of the Li+HF(\hat{v}, \hat{j}) reactive collision for different initial states of the reagent. Journal of Chemical Physics, 1998, 109, 9391-9400.	3.0	64
9	Quantum approaches for the insertion dynamics of the H++D ₂ and D++H ₂ reactive collisions. Journal of Chemical Physics, 2005, 123, 194309.	3.0	61
10	State-to-state reaction probabilities using bond coordinates: Application to the Li+HF(\hat{v}, \hat{j}) collision. Journal of Chemical Physics, 2000, 113, 1781-1794.	3.0	56
11	The lowest triplet state $3\ \hat{A}'\ \hat{e}^2$ of H ₃ ⁺ : Global potential energy surface and vibrational calculations. Journal of Chemical Physics, 2001, 114, 2182-2191.	3.0	53
12	Direct versus resonances mediated F+OH collisions on a new $3\ \hat{A}'\ \hat{e}^3$ potential energy surface. Journal of Chemical Physics, 2004, 121, 4605-4618.	3.0	45
13	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
14	F+OH reactive collisions on new excited $\hat{A}'\ \hat{e}^3$ and $\hat{A}'\ \hat{e}^2$ potential-energy surfaces. Journal of Chemical Physics, 2005, 123, 114310.	3.0	44
15	Accurate fit of the two lowest excited \hat{e}^2 state potential energy surfaces for doublet HeH ₂ ⁺ . Journal of Chemical Physics, 1993, 98, 308-315.	3.0	40
16	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
17	Transition state spectroscopy via infrared excitation of Li \hat{v} 'HF and Li \hat{v} 'DF van der Waals precursors. Journal of Chemical Physics, 1999, 111, 6712-6723.	3.0	39
18	Photodetachment spectrum of OHF[^{sup} \hat{v} ']: Three-dimensional study of the heavy \hat{v} 'light \hat{v} 'heavy resonances. Journal of Chemical Physics, 2004, 121, 309.	3.0	36

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19	Transition state spectroscopy of the excited electronic states of Li ⁺ HF. Journal of Chemical Physics, 2003, 119, 10088-10104.	3.0	35
20	Transition state spectroscopy on the Li-HF system. Journal of Chemical Physics, 1998, 109, 2971-2974.	3.0	32
21	Coupled diabatic potential energy surfaces for studying the nonadiabatic dynamics at conical intersections in angular resolved photodetachment simulations of OHF ⁺ → OHF + e ⁻ . Journal of Chemical Physics, 2006, 125, 164321.	3.0	31
22	Global fit of ab initio potential energy surfaces: II.1. Tetraatomic systems. Computer Physics Communications, 2001, 134, 97-109.	7.5	26
23	Potential energy surfaces and quasiclassical trajectory study of the O + H ₂ → OH + H, OH + H + proton and hydrogen atom transfer reactions and isotopic variants (D ₂ ⁺ , HD ⁺). Physical Chemistry Chemical Physics, 2014, 16, 23594-23603.	2.8	25
24	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
25	Quantum stereodynamics of the F+OH(v, j) reactive collision on the 13A ⁺ state. Molecular Physics, 2004, 102, 2381-2392.	1.7	22
26	Rotation of real spherical harmonics. Computer Physics Communications, 1989, 52, 323-331.	7.5	21
27	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
28	Calculation of two-center one-electron molecular integrals with STOs. Computer Physics Communications, 1991, 64, 329-342.	7.5	19
29	D ₃ +rovibrational levels and spectra for the adiabatic 11A ⁺ and 13A ⁺ electronic states. Physical Chemistry Chemical Physics, 2002, 4, 6012-6017.	2.8	18
30	Analysis of the electronic correlation energy in the LiFH PES using density functional methods. Chemical Physics, 1989, 134, 287-296.	1.9	17
31	Potential energy surface and reactive collisions for the Au+H ₂ system. Journal of Chemical Physics, 2010, 132, 034301.	3.0	16
32	Full dimensional potential energy surface for the ground state of H ₄ ⁺ system based on triatomic-in-molecules formalism. Journal of Chemical Physics, 2013, 139, 184302.	3.0	16
33	Two-configuration mc potential energy surface for the reaction of Mg with HF. Chemical Physics, 1986, 101, 55-65.	1.9	14
34	Ground- and lowest excited-state MRDCI potential-energy surfaces for the collinear Li+HF reaction. Chemical Physics, 1993, 178, 357-362.	1.9	14
35	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
36	Global fit of ab initio potential energy surfaces: II.2. Tetraatomic systems A ₂ B ₂ and ABC ₂ . Computer Physics Communications, 2001, 140, 412-417.	7.5	14

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37	Exploring the transition state for the $\text{Li} + \text{HF} \rightarrow \text{LiF} + \text{H}$ reaction through the $A^1\Sigma^+$ absorption spectrum and $X^1\Sigma^+$ stimulated emission pumping. <i>Journal of Chemical Physics</i> , 2001, 114, 3440-3448.	3.0	14
38	Transition state dynamics of OHF on several electronic states: Photodetachment spectrum of OHF^+ and conical intersections. <i>Journal of Chemical Physics</i> , 2004, 121, 9865-9875.	3.0	14
39	Two-configuration potential energy surface for the collinear $\text{Ca} + \text{HF} \rightarrow \text{CaF} + \text{H}$ reaction. <i>Chemical Physics Letters</i> , 1986, 126, 330-334.	2.6	13
40	The vibrational structure of H_4 and D_4 . <i>Journal of Chemical Physics</i> , 1995, 102, 5725-5732.	3.0	13
41	Basis set convergence of potential energy surfaces: Ground electronic state of H_2 and H . <i>International Journal of Quantum Chemistry</i> , 2011, 111, 387-399.	2.0	12
42	Global nine-dimensional potential energy surface for the H_5 system. II. Fit to an analytical expression. <i>Journal of Chemical Physics</i> , 1999, 110, 7796-7801.	3.0	11
43	Vibrational energy relaxation dynamics of diatomic molecules inside superfluid helium nanodroplets. The case of the H_2 molecule. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 118-130.	2.8	11
44	Accurate and model collinear reactive probabilities of the $\text{Mg} + \text{FH}$ reaction. <i>Chemical Physics Letters</i> , 1990, 168, 441-447.	2.6	10
45	An accurate fit of the potential energy surface of the BeHF system. <i>Computational and Theoretical Chemistry</i> , 1992, 260, 179-193.	1.5	10
46	Relative stability of the $2A_{1g}$ and $2E_g$ states of the C_2H_6^+ ion. <i>Theoretica Chimica Acta</i> , 1979, 53, 377-381.	0.8	8
47	Theoretical study of the ethane ionization spectra within the correlation hole model. <i>Theoretica Chimica Acta</i> , 1979, 54, 53-58.	0.8	7
48	Searching critical points of fitted potential energy surfaces. <i>Computational and Theoretical Chemistry</i> , 1996, 371, 85-90.	1.5	7
49	Application of second-order density functional methods to the calculation of the BeFH potential energy surface. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 491-497.	2.0	7
50	Two-configuration potential energy surface for the $\text{Ca} + \text{HF} \rightarrow \text{CaF} + \text{H}$ reaction. <i>Chemical Physics</i> , 1987, 114, 241-249.	1.9	6
51	Theoretical approach to the structure, energy and electronic spectroscopy of $\text{O} @ (\text{He})_4$ -doped nanodroplets. <i>RSC Advances</i> , 2014, 4, 44972-44979.	3.6	5
52	Dynamics of the $\text{O} + \text{H}_2 \rightarrow \text{OH} + \text{H}$, $\text{OH} + \text{H} \rightarrow \text{H}_2\text{O}$ proton and hydrogen atom transfer reactions on the two lowest potential energy surfaces. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3857-3868.	2.8	5
53	Second-order density functional calculations of the MgFH potential energy surface. <i>Computational and Theoretical Chemistry</i> , 1998, 426, 165-169.	1.5	4
54	Transition state spectroscopy of the excited electronic states of Li^-HF . <i>Chemical Physics Letters</i> , 2002, 351, 295-301.	2.6	4

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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	The potential energy surface of the CaHF system. Computational and Theoretical Chemistry, 1995, 341, 123-132.	1.5	3
57	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