JoÃ£o BrandÃ£o

List of Publications by Year
in descending order

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29	815	759233 12	552781 26
papers	citations	h-index	g-index

29	29	29	307
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quasiclassical study of a termolecular reaction: Application to the HO2 collisional stabilization process. Computational and Theoretical Chemistry, 2022, 1209, 113614.	2.5	2
2	Experimental and theoretical studies of the gas-phase reactions of O(¹D) with H₂O and D₂O at low temperature. Physical Chemistry Chemical Physics, 2021, 23, 25797-25806.	2.8	2
3	A full dimensional potential for H₂O₂(X¹A) covering all dissociation channels. Physical Chemistry Chemical Physics, 2017, 19, 1378-1388.	2.8	7
4	Nâ€dimensional switch function for energy conservation in multiprocess reaction dynamics. Journal of Computational Chemistry, 2016, 37, 1521-1524.	3.3	2
5	The READY program: Building a global potential energy surface and reactive dynamic simulations for the hydrogen combustion. Journal of Computational Chemistry, 2014, 35, 1330-1337.	3.3	4
6	Building symmetric polynomials to fit a potential energy surface: application to an A $$_2$$ 2 B $$_2$$ 2 molecule. Journal of Mathematical Chemistry, 2014, 52, 646-653.	1.5	2
7	Consistent calculation of diabatic energies and diabatic coupling terms in the van der Waals region: Application to the system. Chemical Physics Letters, 2012, 525-526, 160-165.	2.6	0
8	Quasiclassical trajectory calculations of the H+O2 and O+OH reactions on spectroscopically accurate modified DMBE IV PESs. Computational and Theoretical Chemistry, 2010, 946, 2-6.	1.5	3
9	A modified potential for HO2 with spectroscopic accuracy. Journal of Chemical Physics, 2009, 130, 134309.	3.0	10
10	Modelling tunnelling effects in multidimensional quasiclassical trajectories. Application to the O(3P)+H2 reaction. Chemical Physics Letters, 2008, 461, 150-154.	2.6	8
11	An important Well Studied Atmospheric Reaction, <mml:math altimg="si1.gif" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://w. Advances in Quan	0.8	0
12	Dynamical studies and product analysis of O(1D)â€‰+â€‰H2/D2reactions. Molecular Physics, 2007, 105, 359-373.	1.7	12
13	The branching ratio of the O(1D)+HD reaction: A dynamical study. Chemical Physics Letters, 2007, 433, 268-274.	2.6	6
14	Theoretical studies on the O(3P)+H2â†'OH+H reaction. Chemical Physics Letters, 2006, 418, 250-254.	2.6	27
15	Dynamics of the O(P3)+H2 reaction at low temperatures: Comparison of quasiclassical trajectory with quantum scattering calculations. Journal of Chemical Physics, 2006, 124, 074308.	3.0	24
16	Theoretical rate coefficients for the exchange reaction OH+Dâ†'OD+H. Journal of Chemical Physics, 2006, 124, 074305.	3.0	6
17	Potential energy surface for H2O(3Aâ€³) from accurateab initiodata with inclusion of long-range interactions. Journal of Chemical Physics, 2004, 121, 8861-8868.	3.0	34
18	Long-range interactions within the H2O molecule. Chemical Physics Letters, 2003, 372, 866-872.	2.6	16

#	Article	IF	Citations
19	Quasiclassical and capture studies on the O (1D)+H2â†'OH+H reaction using a new potential energy surface for H2O. Chemical Physics Letters, 2003, 377, 523-529.	2.6	20
20	Double-valued potential energy surface for H2O derived from accurateab initiodata and including long-range interactions. Journal of Chemical Physics, 2003, 119, 3148-3159.	3.0	25
21	Quasiclassical trajectory calculations of the thermal rate coefficients for the reactions H(D)+O2â†'OH(D)+O and O+OH(D)â†'O2+H(D) as a function of temperature. Journal of Chemical Physics, 1992, 96, 5137-5150.	3.0	125
22	Recalibration of a single-valued double many-body expansion potential energy surface for ground-state hydroperoxy and dynamics calculations for the oxygen atom + hydroxyl .fwdarw. oxygen + hydrogen atom reaction. The Journal of Physical Chemistry, 1990, 94, 8073-8080.	2.9	244
23	Accurate diatomic curves for Ne2, Ar2, Kr2and Xe2form the extended Hartreeâ€"Fock approximate correlation energy model. Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 1851-1875.	1.1	19
24	A realistic HFACE potential function for Kr2 (X1Î£g+) from spectroscopic and thermophysical data. Computational and Theoretical Chemistry, 1988, 166, 187-192.	1.5	2
25	A realistic hydroperoxo(~X2A") potential energy surface from the double many-body expansion method. The Journal of Physical Chemistry, 1988, 92, 3732-3742.	2.9	83
26	The rational fraction representation of diatomic potentials. Theoretica Chimica Acta, 1987, 71, 459-465.	0.8	8
27	A double many-body expansion of molecular potential energy functions. Molecular Physics, 1986, 57, 387-414.	1.7	57
28	A simple semi-empirical approach to the intermolecular potential of van der Waals systems. Molecular Physics, 1982, 45, 857-875.	1.7	67
29	Internal energy and temperature of a carbon nanotube. Fullerenes Nanotubes and Carbon Nanostructures, 0, , 1-5.	2.1	0