Jose Maria Lucas Alcorta

List of Publications by Year
in descending order

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75 papers	1,517 citations	236833 25 h-index	345118 36 g-index
77 all docs	77 docs citations	77 times ranked	584 citing authors

#	Article	IF	Citations
1	The reactivity of cyclopropyl cyanide in titan's atmosphere: a possible pre-biotic mechanism. Physical Chemistry Chemical Physics, 2018, 20, 6198-6210.	1.3	2
2	The role of Li+ ions in the gas phase dehydrohalogenation and dehydration reactions of i-C3H7Br and i-C3H7OH molecules studied by radiofrequency-guided ion beam techniques and ab initio methods. Journal of Chemical Physics, 2017, 146, 134301.	1.2	0
3	Dehydrohalogenation and Dehydration Reactions ofi-C3H7Br andi-C3H7OH by Sodium Ions Studied by Guided Ion Beam Techniques and Quantum Chemical Methods. Journal of Physical Chemistry A, 2016, 120, 4758-4769.	1.1	2
4	Study by crossed beams and ab initio techniques of an environmentally interesting process: Gas-phase high energy collisions between N2O(1Î£+) and Li+(1S0). Chemical Physics, 2015, 462, 104-110.	0.9	2
5	A molecular dynamics study of the evolution from the formation of the $${ext {C}}_{6}{ext {C}}_{6}{ext {F}}_{6}$$ C 6 F 6 solvation. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	4
6	Experimental and ab initio studies of the reactive processes in gas phase i-C3H7Br and i-C3H7OH collisions with potassium ions. Journal of Chemical Physics, 2014, 141, 164310.	1.2	4
7	Benzeneâ€“Hydrogen Bond (C₆H₆â€“HX) Interactions: The Influence of the X Nature on their Strength and Anisotropy. Journal of Physical Chemistry A, 2014, 118, 1651-1662.	1.1	34
8	Experimental study of the reactive processes in the gas phase K+ + i-C3H7Cl collisions: A comparison with Li and Na ions. Journal of Chemical Physics, 2013, 138, 184310.	1.2	4
9	Crossed molecular beams study of inelastic non-adiabatic processes in gas phase collisions between sodium ions and ZnBr2 molecules in the 0.10â€“3.50 keV energy range. Journal of Chemical Physics, 2012, 137, 154202.	1.2	3
10	Dynamics of alkali ions-neutral molecules reactions: Radio frequency-guided beam experimental cross-sections and direct quasiclassical trajectory studies. AIP Conference Proceedings, 2012, , .	0.3	2
11	Competitive Role of CH₄â€“CH₄ and CHâˆ™Ï€ Interactions in C₆H₆â€“(CH₄)_n Aggregates: The Transition from Dimer to Cluster Features. Journal of Physical Chemistry A, 2012, 116, 5480-5490.	1.1	24
12	Exact activation energies and phenomenological description of quantum tunneling for model potential energy surfaces. The F+H2 reaction at low temperature. Chemical Physics, 2012, 398, 186-191.	0.9	50
13	A 3D-analysis of cluster formation and dynamics of the Xâˆ™-benzene (X = F, Cl, Br, I) ionic dimer solvated by Ar atoms. Physical Chemistry Chemical Physics, 2011, 13, 8251.	1.3	12
14	Exploring the accuracy level of new potential energy surfaces for the F + HD reactions: from exact quantum rate constants to the state-to-state reaction dynamics. Physical Chemistry Chemical Physics, 2011, 13, 8571.	1.3	40
15	Reactive processes in gas phase Na+-iso-C3H7Cl collisions: experimental guided-ion-beam and ab initio studies of the reactions on the ground singlet potential surface of the system up to 12.00 eV. Physical Chemistry Chemical Physics, 2011, 13, 18581.	1.3	5
16	Cross-section energy dependence of the [C6H6â€“M]+ adduct formation between benzene molecules and alkali ions (M = Li, Na, K). Physical Chemistry Chemical Physics, 2011, 13, 15977.	1.3	17
17	A 3D-analysis of the Clâˆ™â€“benzene dimer solvation by Ar atoms. Theoretical Chemistry Accounts, 2011, 128, 757-767.	0.5	8
18	An ab initio theoretical approach to the gas phase decomposition of C₃H₇⁺ produced in ground state Li⁺ + iâ€C₃H₇Cl collisions. International Journal of Quantum Chemistry, 2011, 111, 493-504.	1.0	4

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19	A Generalized Formulation of Ionâ^'Ï€ Electron Interactions: Role of the Nonelectrostatic Component and Probe of the Potential Parameter Transferability. Journal of Physical Chemistry A, 2010, 114, 11964-11970.	1.1	35
20	Experimental cross-sections energy dependence and an ab initio electronic structure survey of the ground singlet potential surface for reactive Li+ + n-C3H7Cl collisions at low energies. Physical Chemistry Chemical Physics, 2010, 12, 13646.	1.3	9
21	An experimental guided-ion-beam andab initiostudy of the ion-molecule gas-phase reactions between Li+ ions andiso-C3H7Cl in their ground electronic state. Journal of Chemical Physics, 2009, 131, 024306.	1.2	11
22	Static and dynamic properties of anionic intermolecular aggregates: the Iâ^'â€“benzeneâ€“Ar n case. Theoretical Chemistry Accounts, 2009, 123, 21-27.	0.5	27
23	Atomâ^'Bond Pairwise Additive Representation for Halideâ^'Benzene Potential Energy Surfaces: an Ab Initio Validation Study. Journal of Physical Chemistry A, 2009, 113, 14606-14614.	1.1	39
24	Guided-Ion-Beam and ab Initio Study of the Li⁺, K⁺, and Rb⁺ Association Reactions with Gas-Phase Butanone and Cyclohexanone in Their Ground Electronic States. Journal of Physical Chemistry A, 2009, 113, 14766-14773.	1.1	7
25	Dynamical study of the Cs+(1S0)+Mg(3Â1S0) non adiabatic collision system in the few keV energy range. European Physical Journal D, 2008, 47, 63-70.	0.6	8
26	Exact state-to-state quantum dynamics of the F+HDâ†'HF(vâ€²=2)+D reaction on model potential energy surfaces. Journal of Chemical Physics, 2008, 129, 064303.	1.2	32
27	A study to improve the van der Waals component of the interaction in water clusters. Physica Scripta, 2008, 78, 058108.	1.2	25
28	Small Water Clusters: The Cases of Rare Gas-Water, Alkali Ion-Water and Water Dimer. Lecture Notes in Computer Science, 2008, , 1026-1035.	1.0	17
29	From Ar Clustering Dynamics to Ar Solvation for Na+â^'Benzene. Journal of Physical Chemistry A, 2007, 111, 1780-1787.	1.1	28
30	Size-Specific Interaction of Alkali Metal Ions in the Solvation of M+â^'Benzene Clusters by Ar Atoms. Journal of Physical Chemistry A, 2007, 111, 8072-8079.	1.1	27
31	Guided ion beams study of ionâ€“molecule reactions at low collision energies: The Li+â€“acetone adduct formation in the 0.10â€“1.00eV center of mass energy range. Chemical Physics Letters, 2007, 442, 28-34.	1.2	16
32	Exact quantum calculations of the kinetic isotope effect: Cross sections and rate constants for the F+HD reaction and role of tunneling. Journal of Chemical Physics, 2006, 125, 133109.	1.2	43
33	Atomâ^'Bond Pairwise Additive Representation for Cationâ^'Benzene Potential Energy Surfaces:â€‰ An ab Initio Validation Study. Journal of Physical Chemistry A, 2006, 110, 9002-9010.	1.1	49
34	Reactive and charge transfer processes in electronically inelastic collisions between ground state cadmium(II) diiodide molecules and lithium ions in the 0.10â€“4.00keV energy range by crossed molecular beams. Chemical Physics Letters, 2006, 425, 234-241.	1.2	9
35	Dynamics of Rb+â€“benzene and Rb+â€“benzeneâ€“Ar (nâ©½ 3) clusters. Chemical Physics, 2006, 328, 221-228.	0.9	24
36	Exact quantum dynamics study of the O++H2(v=0,j=0)â†'OH++H ion-molecule reaction and comparison with quasiclassical trajectory calculations. Journal of Chemical Physics, 2006, 124, 144301.	1.2	29

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37	Benchmark rate constants by the hyperquantization algorithm. The F+H2 reaction for various potential energy surfaces: features of the entrance channel and of the transition state, and low temperature reactivity. Chemical Physics, 2005, 308, 237-253.	0.9	69
38	Inelastic electronic excitation and electron transfer processes in collisions between Mg(3S01) atoms and K+(S01) ions studied by crossed beams in the 0.10-3.80-keV energy range. Journal of Chemical Physics, 2005, 123, 124314.	1.2	10
39	Crossed ionâ€“atom beam study of the inelastic collision processes between neutral Mg(31S0) atoms and Cs+(1S0) ions in the 0.05â€“4.20 keV energy range. Physical Chemistry Chemical Physics, 2005, 7, 310-317.	1.3	12
40	Study ofab initiomolecular data for inelastic and reactive collisions involving the H3+ quasimolecule. Journal of Chemical Physics, 2004, 121, 11629-11638.	1.2	35
41	Lifetime of reactive scattering resonances: Q-matrix analysis and angular momentum dependence for the F+H2 reaction by the hyperquantization algorithm. Journal of Chemical Physics, 2004, 121, 11675-11690.	1.2	64
42	Electronic excitation and charge transfer processes in collisions between Mg(3â€Š1S0) atoms and Rb+(1S0) ions in the 0.07â€“4.00 keV energy range. Journal of Chemical Physics, 2004, 121, 5284-5292.	1.2	12
43	Electron capture processes in collisions between Mg (62S1/2) atoms and Na+(1S0) ions in the 0.10â€“4.00 keV energy range. Chemical Physics Letters, 2003, 382, 106-111.	1.2	9
44	Reactivity enhanced by under-barrier tunneling and resonances: the F+H2â†’HF+H reaction. Chemical Physics Letters, 2003, 371, 504-509.	1.2	42
45	A Quasiclassical Trajectory Study of the Multichannel H(1) + H(2)BO â†’ BO + H2, H(1)BO + H(2), HOB + H Reaction. Journal of Physical Chemistry A, 2003, 107, 1055-1065.	1.1	6
46	An experimental and theoretical study of electronic excitation and charge transfer processes in collisions between Cs() atoms and ions in the 0.30â€“4.00 keV energy range. Chemical Physics, 2002, 281, 33-47.	0.9	8
47	Exact reaction dynamics by the hyperquantization algorithm: integral and differential cross sections for Fâ€‰+â€‰H2, including long-range and spinâ€“orbit effects. Physical Chemistry Chemical Physics, 2002, 4, 401-415.	1.3	72
48	Study of electronic excitation and electron capture processes in the collision between ground-state rubidium atoms and potassium ions by crossed beams. Physical Chemistry Chemical Physics, 2001, 3, 3638-3644.	1.3	13
49	The He + H2+ reaction: a dynamical test on potential energy surfaces for a system exhibiting a pronounced resonance pattern. Chemical Physics Letters, 2000, 318, 619-628.	1.2	70
50	Ab initiodynamics of the He + H⁺₂â†’ HeH⁺+H reaction: a new potential energy surface and quantum mechanical cross-sections. Molecular Physics, 2000, 98, 1835-1849.	0.8	73
51	Anisotropy Effects in Methyl Chloride Ionization by Metastable Neon Atoms at Thermal Energies. Journal of Physical Chemistry A, 2000, 104, 1405-1415.	1.1	26
52	Detailed Energy Dependences of Cross Sections and Rotational Distributions for the Ne + H2+â†’ NeH++ H Reactionâ€. Journal of Physical Chemistry A, 2000, 104, 10227-10233.	1.1	34
53	The application of complex absorbing potentials to an invariant embedding scattering method. II. Applications. Journal of Chemical Physics, 1999, 111, 1979-1987.	1.2	10
54	An experimental study of electronic excitation and electron capture processes in Rb(52S1/2) collision with Cs+ and Li+ ions. Physical Chemistry Chemical Physics, 1999, 1, 5607-5613.	1.3	3

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55	Probabilities for the F+H2â†'HF+H reaction by the hyperquantization algorithm: alternative sequential diagonalization schemes. Physical Chemistry Chemical Physics, 1999, 1, 1091-1098.	1.3	30
56	Exact quantum 3D cross sections for the Ne+H2+â†'NeH++H reaction by the hyperspherical method. Comparison with approximate quantum mechanical and classical results. Physical Chemistry Chemical Physics, 1999, 1, 1125-1132.	1.3	45
57	Rb(52P1/2,3/2) and Rb(62P1/2,3/2) formation in Rb(52S1/2)+Rb+(1S0) collisions by crossed molecular beams. Chemical Physics Letters, 1998, 292, 323-331.	1.2	6
58	Hyperquantization algorithm. II. Implementation for the F+H2 reaction dynamics including open-shell and spin-orbit interactions. Journal of Chemical Physics, 1998, 109, 3805-3818.	1.2	69
59	Electronic excitation and electron capture processes in the collision between Rb atoms and Na ions by crossed molecular beams. Chemical Physics Letters, 1997, 281, 74-80.	1.2	6
60	Electron capture processes in the collision between rubidium ions and sodium neutral atoms by crossed molecular beams. Chemical Physics Letters, 1997, 272, 271-277.	1.2	7
61	Adiabatic and diabatic representations of potential energy curves for the (NaRb)+ system. Chemical Physics Letters, 1996, 261, 583-590.	1.2	13
62	Electronic excitation processes in the collisional system by crossed molecular beams in the 0.1â€"5.0 keV energy range. Chemical Physics, 1996, 209, 217-226.	0.9	8
63	State-to-state crossed molecular beam measurements for collision processes in Na/Na+, K+ and Cs+ systems. Chemical Physics Letters, 1995, 238, 338-345.	1.2	7
64	Threshold Effects and Reaction Barrier in the Li + FH Reaction and Its Isotopic Variants. The Journal of Physical Chemistry, 1995, 99, 11696-11700.	2.9	18
65	Crossed molecular beams study of the M+(1S)+Na(3 2S)â†'M+(1S)+Na(3 2P) collision systems (M+=Li+, Na+,) Tj ETQq1 1 0.784314	1.2	12
66	Calculated versus measured vibrational state specific reactivity of hydrogen atom + fluorine. The Journal of Physical Chemistry, 1993, 97, 8578-8582.	2.9	20
67	Quasiclassical three-dimensional dynamics of the B + OH â†' BO + H reaction : dependence on the nature of the potential-energy surface. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 1587-1592.	1.7	7
68	Heavyâ€"heavyâ€"light limit and exchanged-atom isotopic effects in atomâ€"diatom reactivity. Chemical Physics Letters, 1992, 189, 138-143.	1.2	10
69	Theoretical Characterization of Transition State Dynamical Resonances in Heavyâ€"Lightâ€"Heavy Reactions. Laser Chemistry, 1991, 11, 291-302.	0.5	0
70	Li + HCl RIOSA cross section calculations on parallel computers. Theoretica Chimica Acta, 1991, 79, 191-198.	0.9	13
71	About the convergence of reactive infinite order sudden calculations on parallel computers. Journal of Chemical Physics, 1991, 95, 2218-2219.	1.2	9
72	Hyperspherical study of the collinear C+HFâ†'CH+F reaction. General dynamic behaviour. Chemical Physics, 1989, 136, 115-126.	0.9	2

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73	Dynamical study of the collinear C(3P) + HF(1Î£+)â†'CF(2Î) + H(2S) reaction. Chemical Physics, 1988, 123, 277-293.	0.9	2
74	Theoretical study of the vibrational-rotational spectra of diatomic molecules: A quantum chemistry experiment. Journal of Chemical Education, 1986, 63, 919.	1.1	4
75	Theoretical study of the reaction H + ClCH3 â†' HCl + CH3. Chemical Physics, 1985, 93, 265-275.	0.9	7