

Jose Maria Lucas Alcorta

List of Publications by Year in descending order

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times ranked

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citing authors

#	ARTICLE	IF	CITATIONS
1	Ab initio dynamics of the He + H ₂ ⁺ HeH ⁺ +H reaction: a new potential energy surface and quantum mechanical cross-sections. <i>Molecular Physics</i> , 2000, 98, 1835-1849.	0.8	73
2	Exact reaction dynamics by the hyperquantization algorithm: integral and differential cross sections for F+H ₂ , including long-range and spin-orbit effects. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 401-415.	1.3	72
3	The He + H ₂ ⁺ reaction: a dynamical test on potential energy surfaces for a system exhibiting a pronounced resonance pattern. <i>Chemical Physics Letters</i> , 2000, 318, 619-628.	1.2	70
4	Hyperquantization algorithm. II. Implementation for the F+H ₂ reaction dynamics including open-shell and spin-orbit interactions. <i>Journal of Chemical Physics</i> , 1998, 109, 3805-3818.	1.2	69
5	Benchmark rate constants by the hyperquantization algorithm. The F+H ₂ reaction for various potential energy surfaces: features of the entrance channel and of the transition state, and low temperature reactivity. <i>Chemical Physics</i> , 2005, 308, 237-253.	0.9	69
6	Lifetime of reactive scattering resonances: Q-matrix analysis and angular momentum dependence for the F+H ₂ reaction by the hyperquantization algorithm. <i>Journal of Chemical Physics</i> , 2004, 121, 11675-11690.	1.2	64
7	Exact activation energies and phenomenological description of quantum tunneling for model potential energy surfaces. The F+H ₂ reaction at low temperature. <i>Chemical Physics</i> , 2012, 398, 186-191.	0.9	50
8	Atom-Bond Pairwise Additive Representation for Cation-Benzene Potential Energy Surfaces: An ab Initio Validation Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9002-9010.	1.1	49
9	Exact quantum 3D cross sections for the Ne+H ₂ ⁺ NeH ⁺ +H reaction by the hyperspherical method. Comparison with approximate quantum mechanical and classical results. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 1125-1132.	1.3	45
10	Exact quantum calculations of the kinetic isotope effect: Cross sections and rate constants for the F+HD reaction and role of tunneling. <i>Journal of Chemical Physics</i> , 2006, 125, 133109.	1.2	43
11	Reactivity enhanced by under-barrier tunneling and resonances: the F+H ₂ ⁺ HF+H reaction. <i>Chemical Physics Letters</i> , 2003, 371, 504-509.	1.2	42
12	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. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 8571.	1.3	40
13	Atom-Bond Pairwise Additive Representation for Halide-Benzene Potential Energy Surfaces: an Ab Initio Validation Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14606-14614.	1.1	39
14	Study of ab initio molecular data for inelastic and reactive collisions involving the H ₃ ⁺ quasimolecule. <i>Journal of Chemical Physics</i> , 2004, 121, 11629-11638.	1.2	35
15	A Generalized Formulation of Ion-Electron Interactions: Role of the Nonelectrostatic Component and Probe of the Potential Parameter Transferability. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11964-11970.	1.1	35
16	Detailed Energy Dependences of Cross Sections and Rotational Distributions for the Ne + H ₂ ⁺ NeH ⁺ +H Reaction. <i>Journal of Physical Chemistry A</i> , 2000, 104, 10227-10233.	1.1	34
17	Benzene-Hydrogen Bond (C ₆ H ₆ -HX) Interactions: The Influence of the X Nature on their Strength and Anisotropy. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1651-1662.	1.1	34
18	Exact state-to-state quantum dynamics of the F+HD ⁺ HF(v=2)+D reaction on model potential energy surfaces. <i>Journal of Chemical Physics</i> , 2008, 129, 064303.	1.2	32

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19	Probabilities for the $F+H_2 \rightarrow HF+H$ reaction by the hyperquantization algorithm: alternative sequential diagonalization schemes. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 1091-1098.	1.3	30
20	Exact quantum dynamics study of the $O++H_2(v=0, j=0) \rightarrow OH++H$ ion-molecule reaction and comparison with quasiclassical trajectory calculations. <i>Journal of Chemical Physics</i> , 2006, 124, 144301.	1.2	29
21	From Ar Clustering Dynamics to Ar Solvation for $Na+Ar$ Benzene. <i>Journal of Physical Chemistry A</i> , 2007, 111, 1780-1787.	1.1	28
22	Size-Specific Interaction of Alkali Metal Ions in the Solvation of $M+Ar$ Benzene Clusters by Ar Atoms. <i>Journal of Physical Chemistry A</i> , 2007, 111, 8072-8079.	1.1	27
23	Static and dynamic properties of anionic intermolecular aggregates: the $l^{\sim}benzene^{\sim}Ar_n$ case. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 21-27.	0.5	27
24	Anisotropy Effects in Methyl Chloride Ionization by Metastable Neon Atoms at Thermal Energies. <i>Journal of Physical Chemistry A</i> , 2000, 104, 1405-1415.	1.1	26
25	A study to improve the van der Waals component of the interaction in water clusters. <i>Physica Scripta</i> , 2008, 78, 058108.	1.2	25
26	Dynamics of $Rb+benzene$ and $Rb+benzene^{\sim}Ar$ ($n \in \{1/2, 3\}$) clusters. <i>Chemical Physics</i> , 2006, 328, 221-228.	0.9	24
27	Competitive Role of CH_4 and CH_4^{\sim} Interactions in C_6H_6 (CH_4) _n Aggregates: The Transition from Dimer to Cluster Features. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5480-5490.	1.1	24
28	Calculated versus measured vibrational state specific reactivity of hydrogen atom + fluorine. <i>The Journal of Physical Chemistry</i> , 1993, 97, 8578-8582.	2.9	20
29	Threshold Effects and Reaction Barrier in the $Li + FH$ Reaction and Its Isotopic Variants. <i>The Journal of Physical Chemistry</i> , 1995, 99, 11696-11700.	2.9	18
30	Small Water Clusters: The Cases of Rare Gas-Water, Alkali Ion-Water and Water Dimer. <i>Lecture Notes in Computer Science</i> , 2008, , 1026-1035.	1.0	17
31	Cross-section energy dependence of the $[C_6H_6^{\sim}M]^+$ adduct formation between benzene molecules and alkali ions ($M = Li, Na, K$). <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 15977.	1.3	17
32	Guided ion beams study of ion-molecule reactions at low collision energies: The $Li+acetone$ adduct formation in the 0.10-1.00eV center of mass energy range. <i>Chemical Physics Letters</i> , 2007, 442, 28-34.	1.2	16
33	$Li + HCl$ RIOSA cross section calculations on parallel computers. <i>Theoretica Chimica Acta</i> , 1991, 79, 191-198.	0.9	13
34	Adiabatic and diabatic representations of potential energy curves for the $(NaRb)^+$ system. <i>Chemical Physics Letters</i> , 1996, 261, 583-590.	1.2	13
35	Study of electronic excitation and electron capture processes in the collision between ground-state rubidium atoms and potassium ions by crossed beams. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 3638-3644.	1.3	13
36	Crossed molecular beams study of the $M+(1S)+Na(3 2S) \rightarrow M+(1S)+Na(3 2P)$ collision systems ($M+=Li+, Na+,$) <i>Tj EIQq0 0 0 rgBT /Overl</i>	1.2	12

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37	Electronic excitation and charge transfer processes in collisions between Mg(3s ¹ 1S0) atoms and Rb+(1S0) ions in the 0.07-4.00 keV energy range. Journal of Chemical Physics, 2004, 121, 5284-5292.	1.2	12
38	Crossed ion-atom beam study of the inelastic collision processes between neutral Mg(31S0) atoms and Cs+(1S0) ions in the 0.05-4.20 keV energy range. Physical Chemistry Chemical Physics, 2005, 7, 310-317.	1.3	12
39	A 3D-analysis of cluster formation and dynamics of the X ⁺ -benzene (X = F, Cl, Br, I) ionic dimer solvated by Ar atoms. Physical Chemistry Chemical Physics, 2011, 13, 8251.	1.3	12
40	An experimental guided-ion-beam and ab initio study of the ion-molecule gas-phase reactions between Li+ ions and iso-C ₃ H ₇ Cl in their ground electronic state. Journal of Chemical Physics, 2009, 131, 024306.	1.2	11
41	Heavy-light limit and exchanged-atom isotopic effects in atom-diatom reactivity. Chemical Physics Letters, 1992, 189, 138-143.	1.2	10
42	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
43	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
44	About the convergence of reactive infinite order sudden calculations on parallel computers. Journal of Chemical Physics, 1991, 95, 2218-2219.	1.2	9
45	Electron capture processes in collisions between Mg (62S1/2) atoms and Na+(1S0) ions in the 0.10-4.00 keV energy range. Chemical Physics Letters, 2003, 382, 106-111.	1.2	9
46	Reactive and charge transfer processes in electronically inelastic collisions between ground state cadmium(II) diiodide molecules and lithium ions in the 0.10-4.00keV energy range by crossed molecular beams. Chemical Physics Letters, 2006, 425, 234-241.	1.2	9
47	Experimental cross-sections energy dependence and an ab initio electronic structure survey of the ground singlet potential surface for reactive Li+ + n-C ₃ H ₇ Cl collisions at low energies. Physical Chemistry Chemical Physics, 2010, 12, 13646.	1.3	9
48	Electronic excitation processes in the collisional system by crossed molecular beams in the 0.1-5.0 keV energy range. Chemical Physics, 1996, 209, 217-226.	0.9	8
49	An experimental and theoretical study of electronic excitation and charge transfer processes in collisions between Cs(1) atoms and ions in the 0.30-4.00 keV energy range. Chemical Physics, 2002, 281, 33-47.	0.9	8
50	Dynamical study of the Cs+(1S0)+Mg(3 ¹ S0) non adiabatic collision system in the few keV energy range. European Physical Journal D, 2008, 47, 63-70.	0.6	8
51	A 3D-analysis of the Cl ⁺ -benzene dimer solvation by Ar atoms. Theoretical Chemistry Accounts, 2011, 128, 757-767.	0.5	8
52	Theoretical study of the reaction H + ClCH ₃ → HCl + CH ₃ . Chemical Physics, 1985, 93, 265-275.	0.9	7
53	Quasiclassical three-dimensional dynamics of the B + OH → 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
54	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

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55	Electron capture processes in the collision between rubidium ions and sodium neutral atoms by crossed molecular beams. <i>Chemical Physics Letters</i> , 1997, 272, 271-277.	1.2	7
56	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. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14766-14773.	1.1	7
57	Electronic excitation and electron capture processes in the collision between Rb atoms and Na ions by crossed molecular beams. <i>Chemical Physics Letters</i> , 1997, 281, 74-80.	1.2	6
58	$\text{Rb}(52\text{P}_{1/2,3/2})$ and $\text{Rb}(62\text{P}_{1/2,3/2})$ formation in $\text{Rb}(52\text{S}_{1/2})+\text{Rb}^+(1\text{S}0)$ collisions by crossed molecular beams. <i>Chemical Physics Letters</i> , 1998, 292, 323-331.	1.2	6
59	A Quasiclassical Trajectory Study of the Multichannel $\text{H}(1) + \text{H}(2)\text{BO} \hat{\rightarrow} \text{BO} + \text{H}_2$, $\text{H}(1)\text{BO} + \text{H}(2)$, $\text{HOB} + \text{H}$ Reaction. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1055-1065.	1.1	6
60	Reactive processes in gas phase Na^+ -iso- $\text{C}_3\text{H}_7\text{Cl}$ 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. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18581.	1.3	5
61	Theoretical study of the vibrational-rotational spectra of diatomic molecules: A quantum chemistry experiment. <i>Journal of Chemical Education</i> , 1986, 63, 919.	1.1	4
62	An ab initio theoretical approach to the gas phase decomposition of C_3H_7^+ produced in ground state $\text{Li}^+ + \text{C}_3\text{H}_7\text{Cl}$ collisions. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 493-504.	1.0	4
63	Experimental study of the reactive processes in the gas phase $\text{K}^+ + \text{i-C}_3\text{H}_7\text{Cl}$ collisions: A comparison with Li and Na ions. <i>Journal of Chemical Physics</i> , 2013, 138, 184310.	1.2	4
64	Experimental and ab initio studies of the reactive processes in gas phase $\text{i-C}_3\text{H}_7\text{Br}$ and $\text{i-C}_3\text{H}_7\text{OH}$ collisions with potassium ions. <i>Journal of Chemical Physics</i> , 2014, 141, 164310.	1.2	4
65	A molecular dynamics study of the evolution from the formation of the C_6F_6 solvation. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	4
66	An experimental study of electronic excitation and electron capture processes in $\text{Rb}(52\text{S}_{1/2})$ collision with Cs^+ and Li^+ ions. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 5607-5613.	1.3	3
67	Crossed molecular beams study of inelastic non-adiabatic processes in gas phase collisions between sodium ions and ZnBr_2 molecules in the 0.10–3.50 keV energy range. <i>Journal of Chemical Physics</i> , 2012, 137, 154202.	1.2	3
68	Dynamical study of the collinear $\text{C}(3\text{P}) + \text{HF}(1^1\Sigma^+) \hat{\rightarrow} \text{CF}(2^1\Sigma^+) + \text{H}(2\text{S})$ reaction. <i>Chemical Physics</i> , 1988, 123, 277-293.	0.9	2
69	Hyperspherical study of the collinear $\text{C}+\text{HF} \hat{\rightarrow} \text{CH}+\text{F}$ reaction. General dynamic behaviour. <i>Chemical Physics</i> , 1989, 136, 115-126.	0.9	2
70	Dynamics of alkali ions-neutral molecules reactions: Radio frequency-guided beam experimental cross-sections and direct quasiclassical trajectory studies. <i>AIP Conference Proceedings</i> , 2012, , .	0.3	2
71	Study by crossed beams and ab initio techniques of an environmentally interesting process: Gas-phase high energy collisions between $\text{N}_2\text{O}(1^1\Sigma^+)$ and $\text{Li}^+(1\text{S}0)$. <i>Chemical Physics</i> , 2015, 462, 104-110.	0.9	2
72	Dehydrohalogenation and Dehydration Reactions of $\text{i-C}_3\text{H}_7\text{Br}$ and $\text{i-C}_3\text{H}_7\text{OH}$ by Sodium Ions Studied by Guided Ion Beam Techniques and Quantum Chemical Methods. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4758-4769.	1.1	2

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73	The reactivity of cyclopropyl cyanide in titan's atmosphere: a possible pre-biotic mechanism. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 6198-6210.	1.3	2
74	Theoretical Characterization of Transition State Dynamical Resonances in Heavy-“Light”-Heavy Reactions. <i>Laser Chemistry</i> , 1991, 11, 291-302.	0.5	0
75	The role of Li ⁺ ions in the gas phase dehydrohalogenation and dehydration reactions of i-C ₃ H ₇ Br and i-C ₃ H ₇ OH molecules studied by radiofrequency-guided ion beam techniques and ab initio methods. <i>Journal of Chemical Physics</i> , 2017, 146, 134301.	1.2	0