Ernesto Garcia

List of Publications by Year
in descending order

95 papers	1,825 citations	257450 24 h-index	330143 37 g-index
96 all docs	96 docs citations	96 times ranked	532 citing authors

#	Article	IF	Citations
1	Temperature dependence of the rate coefficient of formation of CN radical from CÂ+ÂNH. Chemical Physics Letters, 2021, 771, 138493.	2.6	1
2	Collisional O2 + N2 State-Selected Cross Sections for Open Science Cloud Reuse. Journal of Physical Chemistry A, 2020, 124, 6445-6457.	2.5	2
3	Kinetics Of The H + CH₂ â†' CH + H₂ Reaction At Low Temperature. Journal of Physical Chemistry A, 2019, 123, 7408-7419.	2.5	5
4	How reactant polarization can be used to change the effect of interference on reactive collisions. Physical Chemistry Chemical Physics, 2019, 21, 14012-14022.	2.8	9
5	Î›-Doublet Propensities for Reactions on Competing Aâ€² and Aâ€³ Potential Energy Surfaces: O(³P) + N₂ and O(³P) + HCl. Journal of Physical Chemistry A, 2018, 122, 2739-2750.	2.5	5
6	Comparisons and scaling rules between N+N₂and N₂+N₂collision induced dissociation cross sections from atomistic studies. Plasma Sources Science and Technology, 2017, 26, 045005.	3.1	17
7	Closer versus Long Range Interaction Effects on the Non-Arrhenius Behavior of Quasi-Resonant O₂ + N₂ Collisions. Journal of Physical Chemistry A, 2017, 121, 5088-5099.	2.5	4
8	The role of the long-range tail of the potential in O₂ + N₂ collisional inelastic vibrational energy transfers. Physical Chemistry Chemical Physics, 2017, 19, 11206-11211.	2.8	10
9	Impact of the Long-Range Interaction on the Efficiency of the Li + ClH â†' LiCl + H Reaction. Journal of Physical Chemistry A, 2017, 121, 6349-6356.	2.5	6
10	On the temperature dependence of the rate coefficient of formation of C$_2^+$ from C + CH⁺. Monthly Notices of the Royal Astronomical Society, 2016, 460, 2368-2375.	4.4	20
11	A Dynamics Investigation of the C + CH⁺â†' C₂⁺+ H Reaction on an ab Initio Bond-Order-Like Potential. Journal of Physical Chemistry A, 2016, 120, 5125-5135.	2.5	15
12	Enhanced Flexibility of the O₂ + N₂ Interaction and Its Effect on Collisional Vibrational Energy Exchange. Journal of Physical Chemistry A, 2016, 120, 5208-5219.	2.5	10
13	Efficiency of Collisional O₂ + N₂ Vibrational Energy Exchange. Journal of Physical Chemistry B, 2016, 120, 1476-1485.	2.6	20
14	Quasi-resonant vibrational energy transfer in N2+N2 collisions: Effect of the long-range interaction. Chemical Physics Letters, 2015, 620, 103-108.	2.6	20
15	The effect of the intermolecular potential formulation on the stateâ€selected energy exchange rate coefficients in N₂â€"N₂ collisions. Journal of Computational Chemistry, 2014, 35, 722-736.	3.3	17
16	Understanding the reaction between muonium atoms and hydrogen molecules: zero point energy, tunnelling, and vibrational adiabaticity. Molecular Physics, 2013, 111, 3169-3181.	1.7	22
17	Dynamics of the reactions of muonium and deuterium atoms with vibrationally excited hydrogen molecules: tunneling and vibrational adiabaticity. Physical Chemistry Chemical Physics, 2012, 14, 14596.	2.8	24
18	An innovative computational comparison of exact and centrifugal sudden quantum properties of the N + N₂reaction. Physical Chemistry Chemical Physics, 2012, 14, 1589-1595.	2.8	4

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19	A classical versus quantum mechanics study of the $$hbox{OH},+,hbox{CO} ightarrow,hbox{H},+,hbox{CO}_2$$ (JÂ=Â0) reaction. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	4
20	A detailed product distribution analysis of some potential energy surfaces describing the OH+COâ†'H+CO2 reaction. Computational and Theoretical Chemistry, 2012, 990, 47-52.	2.5	15
21	The last mile of molecular reaction dynamics virtual experiments: the case of the OH(N = 1â€“10) + CO(j =) Tj ETQq1 1 0.784314 rgB	3.2	28
22	Capture and dissociation in the complex-forming CH(v = 0,1) + D2â†' CHD + D, CD2 + H, CD + HD reactions and comparison with CH(v = 0,1) + H2. Physical Chemistry Chemical Physics, 2011, 13, 13638.	2.8	2
23	Capture and dissociation in the complex-forming CH+H2â†' CH2+H, CH+H2 reactions. Physical Chemistry Chemical Physics, 2011, 13, 3421.	2.8	12
24	Can quasiclassical trajectory calculations reproduce the extreme kinetic isotope effect observed in the muonic isotopologues of the H + H2 reaction?. Journal of Chemical Physics, 2011, 135, 034310.	3.0	25
25	On the anomaly of the quasiclassical product distributions of the $$hbox{OH} +hbox{CO} ightarrowhbox{H} +hbox{CO}_2$$ reaction. Theoretical Chemistry Accounts, 2011, 128, 727-734.	1.4	8
26	An Extension of the Molecular Simulator GEMS to Calculate the Signal of Crossed Beam Experiments. Lecture Notes in Computer Science, 2011, , 453-465.	1.3	14
27	A study of the impact of long range interactions on the reactivity of N + N<SUB align=right>2 using the Grid Empowered Molecular Simulator GEMS. International Journal of Web and Grid Services, 2010, 6, 196.	0.5	11
28	Accurate Quantum Dynamics on Grid Platforms: Some Effects of Long Range Interactions on the Reactivity of N + N2. Lecture Notes in Computer Science, 2010, , 1-12.	1.3	6
29	Effect of the Total Angular Momentum on the Dynamics of the H₂ + H₂ System. Journal of Physical Chemistry A, 2009, 113, 14312-14320.	2.5	7
30	A detailed comparison of centrifugal sudden and J-shift estimates of the reactive properties of the N + N2 reaction. Physical Chemistry Chemical Physics, 2009, 11, 11456.	2.8	10
31	A comparison of the quantum state-specific efficiency of N + N2 reaction computed on different potential energy surfaces. Physical Chemistry Chemical Physics, 2009, 11, 1752.	2.8	30
32	A Comparison of the Isotope Effect for the N + N2 Reaction Calculated on Two Potential Energy Surfaces. Lecture Notes in Computer Science, 2008, , 1081-1093.	1.3	11
33	Modeling the global potential energy surface of the N + N2 reaction from ab initio data. Physical Chemistry Chemical Physics, 2008, 10, 2552.	2.8	39
34	Thermal rate coefficients in collinear versus bent transition state reactions: the N+N₂case study. Physica Scripta, 2008, 78, 058116.	2.5	25
35	Grid Computing in Time-Dependent Quantum Reactive Dynamics. Lecture Notes in Computer Science, 2008, , 1065-1080.	1.3	6
36	The Shape of the Potential Energy Surface and the Thermal Rate Coefficients of the N + N₂ Reaction. Journal of Physical Chemistry A, 2007, 111, 10362-10368.	2.5	15

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37	A detailed trajectory study of the OH+COâ†'H+CO2 reaction. Chemical Physics, 2007, 332, 162-175.	1.9	21
38	Theoretical Study of the Complex-Forming CH + H2â†' CH2+ H Reactionâ€. Journal of Physical Chemistry A, 2006, 110, 5542-5548.	2.5	16
39	Invariant energy partitions in chemical reactions and cluster dynamics simulations. Computational Materials Science, 2006, 35, 187-191.	3.0	29
40	Calculated versus measured product distributions of the OH+D 2 reaction. Molecular Physics, 2006, 104, 839-846.	1.7	9
41	MEP-MPE potential energy surface for the Cl + CH4 â†' HCl + CH3 reaction. International Journal of Quantum Chemistry, 2006, 106, 623-630.	2.0	6
42	A multiproperty analysis of the OH+H2(D2,HD) potential energy surface. Chemical Physics, 2005, 308, 201-210.	1.9	7
43	Thermal Rate Coefficients for the N + N 2 Reaction: Quasiclassical, Semiclassical and Quantum Calculations. Lecture Notes in Computer Science, 2005, , 1083-1092.	1.3	4
44	Bond Order Potentials for a priori Simulations of Polyatomic Reactions. Lecture Notes in Computer Science, 2004, , 328-337.	1.3	3
45	A Full Dimensional Quasiclassical Trajectory Study of Cl + CH4Rate Coefficientsâ€. Journal of Physical Chemistry A, 2004, 108, 8752-8758.	2.5	15
46	Isotopic effects in the product vibrational distribution of the OH(OD)+HCl reaction. Chemical Physics Letters, 2003, 371, 223-228.	2.6	10
47	A LAGROBO Multiproperty Fit to Four-Atom Potential Energy Surfaces:â€‰ The OH + HCl Case Study. Journal of Physical Chemistry A, 2003, 107, 7248-7257.	2.5	9
48	Quasiclassical Rate Coefficients for the H2+H2 Reaction and Dissociation. Journal of Physical and Chemical Reference Data, 2002, 31, 371-385.	4.2	18
49	Reaction and dissociation mechanism control: the H2â€‰+â€‰H2system. Physical Chemistry Chemical Physics, 2002, 4, 5007-5013.	2.8	9
50	A LAGROBO strategy to fit potential energy surfaces: the OH+HCl reaction. Chemical Physics Letters, 2002, 360, 304-312.	2.6	27
51	Quasiclassical Kinetics of the H2 + H2 Reaction and Dissociation. Journal of Physical Chemistry A, 2001, 105, 1797-1804.	2.5	17
52	A trajectory study of the OH+H2 reaction. Chemical Physics Letters, 2001, 333, 471-478.	2.6	13
53	Progress in validating the potential energy surface of the OH+H2 reaction: product vibrational distributions. Chemical Physics Letters, 2001, 345, 219-227.	2.6	12
54	A Quasiclassical Trajectory Study of Atom Diatom Reactions. Lecture Notes in Quantum Chemistry II, 2000, , 242-256.	0.3	0

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55	A quasiclassical trajectory study of the H2+H2 reaction. Chemical Physics Letters, 1999, 305, 276-284.	2.6	24
56	On multiquantum vibrational deexcitation in symmetric reactions. Chemical Physics Letters, 1998, 288, 616-620.	2.6	12
57	The largest angle generalization of the rotating bond order potential: Three different atom reactions. Journal of Chemical Physics, 1998, 108, 3886-3896.	3.0	58
58	Rate coefficients under jet conditions. Plasma Sources Science and Technology, 1998, 7, 359-362.	3.1	5
59	Ab initio calculations and dynamical tests of a potential energy surface for the Na+FH reaction. Journal of Chemical Physics, 1997, 106, 10222-10229.	3.0	27
60	Accurate calculations of cross sections and rate coefficients of some atom - diatom reactions relevant to plasma chemistry. Plasma Sources Science and Technology, 1997, 6, 270-279.	3.1	6
61	Effect of Varying the Transition State Geometry on N + N2Vibrational Deexcitation Rate Coefficients. Journal of Physical Chemistry A, 1997, 101, 4734-4740.	2.5	33
62	Reactive Vibrational Deexcitation: The N + N2 and O + O2 Reactions. , 1996, , 35-52.		7
63	Theoretical Study of the O(1D) + HCl Reaction on a Model Potential. The Journal of Physical Chemistry, 1995, 99, 17139-17144.	2.9	39
64	The largest angle generalization of the rotating bond order potential: The H+H2and N+N2reactions. Journal of Chemical Physics, 1995, 103, 5410-5416.	3.0	40
65	Temperature dependence of quasiclassical and quantum rate coefficients for N + N2. , 1994, , .		1
66	Temperature dependence of nitrogen atom-molecule rate coefficients. The Journal of Physical Chemistry, 1994, 98, 502-507.	2.9	100
67	Cooperative mechanisms for the Hâ€,+â€,ICl reaction and their significance for the Kâ€,+â€,ICl experiment. Canadian Journal of Chemistry, 1994, 72, 919-927.	1.1	3
68	Potential energy representations in the bond order space. Chemical Physics, 1992, 168, 341-348.	1.9	30
69	Deactivation dynamics of vibrationally excited nitrogen molecules by nitrogen atoms. Effects on non-equilibrium vibrational distribution and dissociation rates of nitrogen under electrical discharges. Chemical Physics Letters, 1992, 200, 597-604.	2.6	82
70	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
71	Parallel calculations of quasiclassical rate constants: the H + H2 reaction. Chemical Physics Letters, 1991, 176, 273-279.	2.6	6
72	Parallel calculations of approximate 3D quantum cross sections: the Li + HF reaction. Chemical Physics Letters, 1991, 176, 280-286.	2.6	18

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73	D+D 2 Quasiclassical rate constant calculations on parallel computers. Theoretica Chimica Acta, 1991, 79, 323-333.	0.8	8
74	A modelling of accurate reduced-dimensionality quantum probabilities for H(D,T)+Cl2 reactions. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1990, 12, 1539-1551.	0.4	5
75	Calculated vs measured scattering and kinetic data for the Li+HCl reaction. Journal of Chemical Physics, 1990, 93, 8764-8770.	3.0	12
76	An approximate three-dimensional quantum-mechanical study of the Li+HFâ†'LiF+H reaction. Chemical Physics Letters, 1989, 158, 362-368.	2.6	14
77	Approximate Quantum Techniques for Atom Diatom Reactions. , 1989, , 271-294.		6
78	Quasiclassical Calculations for Alkali and Alkaline Earth + Hydrogen Halide Chemical Reactions Using Supercomputers. , 1989, , 383-393.		2
79	A bond-order LiFH potential energy surface for 3D quantum-mechanical calculations. Chemical Physics Letters, 1988, 143, 174-180.	2.6	40
80	A potential energy surface for the Li+HCl reaction. Journal of Chemical Physics, 1988, 88, 181-190.	3.0	30
81	Improved infinite order sudden cross sections for the Li+HF reaction. Journal of Chemical Physics, 1988, 89, 7238-7241.	3.0	34
82	Deactivation of vibrationally excited nitrogen molecules by collision with nitrogen atoms. The Journal of Physical Chemistry, 1987, 91, 312-314.	2.9	130
83	A vectorizable potential energy functional for reactive scattering. Theoretica Chimica Acta, 1987, 72, 253-264.	0.8	13
84	An approximate estimate of the Li+HF reactivity. Chemical Physics Letters, 1987, 139, 140-144.	2.6	13
85	Title is missing!. The Journal of Physical Chemistry, 1986, 90, 987-989.	2.9	14
86	Rate constants for the deactivation of thermal (T = 300 k) H2 molecules by hydrogen atoms. Chemical Physics Letters, 1986, 123, 365-370.	2.6	29
87	On the transition state of the Li + Hcl reaction. Chemical Physics Letters, 1986, 127, 73-77.	2.6	15
88	An improvement of the Li+HF PES based on a 3D quasiclassical trajectory test. Journal of Chemical Physics, 1986, 84, 3059-3067.	3.0	43
89	Selective tunnelling effects in collinear chemical reactions. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1985, 5, 541-550.	0.4	7
90	A quantum-mechanical test for a LiHCl semi-empirical surface. Chemical Physics Letters, 1985, 120, 75-79.	2.6	12

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91	A new bond-order functional form for triatomic molecules. Molecular Physics, 1985, 56, 629-639.	1.7	69
92	Diatomic potential functions for triatomic scattering. Molecular Physics, 1985, 56, 621-627.	1.7	60
93	A fit of the potential energy surface of the LiHF system. Molecular Physics, 1984, 52, 1115-1124.	1.7	41
94	A smooth potential energy fit for reactive systems. Computational and Theoretical Chemistry, 1984, 107, 91-94.	1.5	7
95	Franck-Condon factors and R-centroids for the A1âˆ'+-X1âˆ'+ and B3Î(0+)â€™X1âˆ'+ band system of 63Cu1H and 63Cu2H. Journal of Quantitative Spectroscopy and Radiative Transfer, 1983, 30, 439-447.	2.3	1