

# Ernesto Garcia

## List of Publications by Year in descending order

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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	Deactivation of vibrationally excited nitrogen molecules by collision with nitrogen atoms. The Journal of Physical Chemistry, 1987, 91, 312-314.	2.9	130
2	Temperature dependence of nitrogen atom-molecule rate coefficients. The Journal of Physical Chemistry, 1994, 98, 502-507.	2.9	100
3	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
4	A new bond-order functional form for triatomic molecules. Molecular Physics, 1985, 56, 629-639.	1.7	69
5	Diatomic potential functions for triatomic scattering. Molecular Physics, 1985, 56, 621-627.	1.7	60
6	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
7	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
8	A fit of the potential energy surface of the LiHF system. Molecular Physics, 1984, 52, 1115-1124.	1.7	41
9	A bond-order LiFH potential energy surface for 3D quantum-mechanical calculations. Chemical Physics Letters, 1988, 143, 174-180.	2.6	40
10	The largest angle generalization of the rotating bond order potential: The H+H <sub>2</sub> and N+N <sub>2</sub> reactions. Journal of Chemical Physics, 1995, 103, 5410-5416.	3.0	40
11	Theoretical Study of the O(1D) + HCl Reaction on a Model Potential. The Journal of Physical Chemistry, 1995, 99, 17139-17144.	2.9	39
12	Modeling the global potential energy surface of the N + N <sub>2</sub> reaction from ab initio data. Physical Chemistry Chemical Physics, 2008, 10, 2552.	2.8	39
13	Improved infinite order sudden cross sections for the Li+HF reaction. Journal of Chemical Physics, 1988, 89, 7238-7241.	3.0	34
14	Effect of Varying the Transition State Geometry on N + N <sub>2</sub> Vibrational Deexcitation Rate Coefficients. Journal of Physical Chemistry A, 1997, 101, 4734-4740.	2.5	33
15	A potential energy surface for the Li+HCl reaction. Journal of Chemical Physics, 1988, 88, 181-190.	3.0	30
16	Potential energy representations in the bond order space. Chemical Physics, 1992, 168, 341-348.	1.9	30
17	A comparison of the quantum state-specific efficiency of N + N <sub>2</sub> reaction computed on different potential energy surfaces. Physical Chemistry Chemical Physics, 2009, 11, 1752.	2.8	30
18	Rate constants for the deactivation of thermal (T = 300 k) H <sub>2</sub> molecules by hydrogen atoms. Chemical Physics Letters, 1986, 123, 365-370.	2.6	29

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19	Invariant energy partitions in chemical reactions and cluster dynamics simulations. Computational Materials Science, 2006, 35, 187-191.	3.0	29
20	The last mile of molecular reaction dynamics virtual experiments: the case of the OH(N = 1) + CO(j = 1) reaction. Journal of Chemical Physics, 2006, 125, 084301.	3.2	28
21	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
22	A LAGROBO strategy to fit potential energy surfaces: the OH+HCl reaction. Chemical Physics Letters, 2002, 360, 304-312.	2.6	27
23	Thermal rate coefficients in collinear versus bent transition state reactions: the N+N <sub>2</sub> case study. Physica Scripta, 2008, 78, 058116.	2.5	25
24	Can quasiclassical trajectory calculations reproduce the extreme kinetic isotope effect observed in the muonic isotopologues of the H + H <sub>2</sub> reaction?. Journal of Chemical Physics, 2011, 135, 034310.	3.0	25
25	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
26	A quasiclassical trajectory study of the H <sub>2</sub> +H <sub>2</sub> reaction. Chemical Physics Letters, 1999, 305, 276-284.	2.6	24
27	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
28	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
29	A detailed trajectory study of the OH+CO <sup>+</sup> H+CO <sub>2</sub> reaction. Chemical Physics, 2007, 332, 162-175.	1.9	21
30	Quasi-resonant vibrational energy transfer in N <sub>2</sub> +N <sub>2</sub> collisions: Effect of the long-range interaction. Chemical Physics Letters, 2015, 620, 103-108.	2.6	20
31	On the temperature dependence of the rate coefficient of formation of C <sub>2</sub> <sup>+</sup> from C + CH <sup>+</sup> . Monthly Notices of the Royal Astronomical Society, 2016, 460, 2368-2375.	4.4	20
32	Efficiency of Collisional O <sub>2</sub> + N <sub>2</sub> Vibrational Energy Exchange. Journal of Physical Chemistry B, 2016, 120, 1476-1485.	2.6	20
33	Parallel calculations of approximate 3D quantum cross sections: the Li + HF reaction. Chemical Physics Letters, 1991, 176, 280-286.	2.6	18
34	Quasiclassical Rate Coefficients for the H <sub>2</sub> +H <sub>2</sub> Reaction and Dissociation. Journal of Physical and Chemical Reference Data, 2002, 31, 371-385.	4.2	18
35	Quasiclassical Kinetics of the H <sub>2</sub> + H <sub>2</sub> Reaction and Dissociation. Journal of Physical Chemistry A, 2001, 105, 1797-1804.	2.5	17
36	The effect of the intermolecular potential formulation on the state-selected energy exchange rate coefficients in N <sub>2</sub> +N <sub>2</sub> collisions. Journal of Computational Chemistry, 2014, 35, 722-736.	3.3	17

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37	Comparisons and scaling rules between $N+N_2$ and $N_2+N_2$ collision induced dissociation cross sections from atomistic studies. <i>Plasma Sources Science and Technology</i> , 2017, 26, 045005.	3.1	17
38	Theoretical Study of the Complex-Forming $CH + H_2 \rightarrow CH_2 + H$ Reaction. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5542-5548.	2.5	16
39	On the transition state of the $Li + HCl$ reaction. <i>Chemical Physics Letters</i> , 1986, 127, 73-77.	2.6	15
40	A Full Dimensional Quasiclassical Trajectory Study of $Cl + CH_4$ Rate Coefficients. <i>Journal of Physical Chemistry A</i> , 2004, 108, 8752-8758.	2.5	15
41	The Shape of the Potential Energy Surface and the Thermal Rate Coefficients of the $N + N_2$ Reaction. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10362-10368.	2.5	15
42	A detailed product distribution analysis of some potential energy surfaces describing the $OH+CO \rightarrow H+CO_2$ reaction. <i>Computational and Theoretical Chemistry</i> , 2012, 990, 47-52.	2.5	15
43	A Dynamics Investigation of the $C + CH^+ \rightarrow C_2^+ + H$ Reaction on an ab Initio Bond-Order-Like Potential. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5125-5135.	2.5	15
44	Title is missing!. <i>The Journal of Physical Chemistry</i> , 1986, 90, 987-989.	2.9	14
45	An approximate three-dimensional quantum-mechanical study of the $Li+HF \rightarrow LiF+H$ reaction. <i>Chemical Physics Letters</i> , 1989, 158, 362-368.	2.6	14
46	An Extension of the Molecular Simulator GEMS to Calculate the Signal of Crossed Beam Experiments. <i>Lecture Notes in Computer Science</i> , 2011, , 453-465.	1.3	14
47	A vectorizable potential energy functional for reactive scattering. <i>Theoretica Chimica Acta</i> , 1987, 72, 253-264.	0.8	13
48	An approximate estimate of the $Li+HF$ reactivity. <i>Chemical Physics Letters</i> , 1987, 139, 140-144.	2.6	13
49	A trajectory study of the $OH+H_2$ reaction. <i>Chemical Physics Letters</i> , 2001, 333, 471-478.	2.6	13
50	A quantum-mechanical test for a $LiHCl$ semi-empirical surface. <i>Chemical Physics Letters</i> , 1985, 120, 75-79.	2.6	12
51	Calculated vs measured scattering and kinetic data for the $Li+HCl$ reaction. <i>Journal of Chemical Physics</i> , 1990, 93, 8764-8770.	3.0	12
52	On multiquantum vibrational deexcitation in symmetric reactions. <i>Chemical Physics Letters</i> , 1998, 288, 616-620.	2.6	12
53	Progress in validating the potential energy surface of the $OH+H_2$ reaction: product vibrational distributions. <i>Chemical Physics Letters</i> , 2001, 345, 219-227.	2.6	12
54	Capture and dissociation in the complex-forming $CH+H_2 \rightarrow CH_2+H$ , $CH+H_2$ reactions. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 3421.	2.8	12

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55	A Comparison of the Isotope Effect for the N + N <sub>2</sub> Reaction Calculated on Two Potential Energy Surfaces. Lecture Notes in Computer Science, 2008, , 1081-1093.	1.3	11
56	A study of the impact of long range interactions on the reactivity of N + N <sub>2</sub> using the Grid Empowered Molecular Simulator GEMS. International Journal of Web and Grid Services, 2010, 6, 196.	0.5	11
57	Isotopic effects in the product vibrational distribution of the OH(OD)+HCl reaction. Chemical Physics Letters, 2003, 371, 223-228.	2.6	10
58	A detailed comparison of centrifugal sudden and J-shift estimates of the reactive properties of the N + N <sub>2</sub> reaction. Physical Chemistry Chemical Physics, 2009, 11, 11456.	2.8	10
59	Enhanced Flexibility of the O <sub>2</sub> + N <sub>2</sub> Interaction and Its Effect on Collisional Vibrational Energy Exchange. Journal of Physical Chemistry A, 2016, 120, 5208-5219.	2.5	10
60	The role of the long-range tail of the potential in O <sub>2</sub> + N <sub>2</sub> collisional inelastic vibrational energy transfers. Physical Chemistry Chemical Physics, 2017, 19, 11206-11211.	2.8	10
61	Reaction and dissociation mechanism control: the H <sub>2</sub> +H <sub>2</sub> system. Physical Chemistry Chemical Physics, 2002, 4, 5007-5013.	2.8	9
62	A LAGROBO Multiproperty Fit to Four-Atom Potential Energy Surfaces: The OH + HCl Case Study. Journal of Physical Chemistry A, 2003, 107, 7248-7257.	2.5	9
63	Calculated versus measured product distributions of the OH+D <sub>2</sub> reaction. Molecular Physics, 2006, 104, 839-846.	1.7	9
64	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
65	D+D <sub>2</sub> Quasiclassical rate constant calculations on parallel computers. Theoretica Chimica Acta, 1991, 79, 323-333.	0.8	8
66	On the anomaly of the quasiclassical product distributions of the $\text{OH} + \text{CO} \rightarrow \text{H} + \text{CO}_2$ reaction. Theoretical Chemistry Accounts, 2011, 128, 727-734.	1.4	8
67	A smooth potential energy fit for reactive systems. Computational and Theoretical Chemistry, 1984, 107, 91-94.	1.5	7
68	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
69	Reactive Vibrational Deexcitation: The N + N <sub>2</sub> and O + O <sub>2</sub> Reactions. , 1996, , 35-52.		7
70	A multiproperty analysis of the OH+H <sub>2</sub> (D <sub>2</sub> ,HD) potential energy surface. Chemical Physics, 2005, 308, 201-210.	1.9	7
71	Effect of the Total Angular Momentum on the Dynamics of the H <sub>2</sub> + H <sub>2</sub> System. Journal of Physical Chemistry A, 2009, 113, 14312-14320.	2.5	7
72	Parallel calculations of quasiclassical rate constants: the H + H <sub>2</sub> reaction. Chemical Physics Letters, 1991, 176, 273-279.	2.6	6

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73	Accurate calculations of cross sections and rate coefficients of some atom - diatom reactions relevant to plasma chemistry. <i>Plasma Sources Science and Technology</i> , 1997, 6, 270-279.	3.1	6
74	MEP-MPE potential energy surface for the $\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3$ reaction. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 623-630.	2.0	6
75	Impact of the Long-Range Interaction on the Efficiency of the $\text{Li} + \text{ClH} \rightarrow \text{LiCl} + \text{H}$ Reaction. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6349-6356.	2.5	6
76	Grid Computing in Time-Dependent Quantum Reactive Dynamics. <i>Lecture Notes in Computer Science</i> , 2008, , 1065-1080.	1.3	6
77	Accurate Quantum Dynamics on Grid Platforms: Some Effects of Long Range Interactions on the Reactivity of $\text{N} + \text{N}_2$ . <i>Lecture Notes in Computer Science</i> , 2010, , 1-12.	1.3	6
78	Approximate Quantum Techniques for Atom Diatom Reactions. , 1989, , 271-294.		6
79	A modelling of accurate reduced-dimensionality quantum probabilities for $\text{H(D,T)} + \text{Cl}_2$ reactions. <i>Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics</i> , 1990, 12, 1539-1551.	0.4	5
80	Rate coefficients under jet conditions. <i>Plasma Sources Science and Technology</i> , 1998, 7, 359-362.	3.1	5
81	$\hat{1}$ -Doublet Propensities for Reactions on Competing $\langle i \rangle \text{A} \langle /i \rangle \hat{\text{e}}^2$ and $\langle i \rangle \text{A} \langle /i \rangle \hat{\text{e}}^3$ Potential Energy Surfaces: $\text{O}(\langle \text{sup} \rangle 3 \langle /sup \rangle \langle i \rangle \text{P} \langle /i \rangle) + \text{N} \langle \text{sub} \rangle 2 \langle /sub \rangle$ and $\text{O}(\langle \text{sup} \rangle 3 \langle /sup \rangle \langle i \rangle \text{P} \langle /i \rangle) + \text{HCl}$ . <i>Journal of Physical Chemistry A</i> , 2018, 122, 2739-2750.	2.5	5
82	Kinetics Of The $\text{H} + \text{CH} \langle \text{sub} \rangle 2 \langle /sub \rangle \hat{\text{t}}' \text{CH} + \text{H} \langle \text{sub} \rangle 2 \langle /sub \rangle$ Reaction At Low Temperature. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7408-7419.	2.5	5
83	Thermal Rate Coefficients for the $\text{N} + \text{N}_2$ Reaction: Quasiclassical, Semiclassical and Quantum Calculations. <i>Lecture Notes in Computer Science</i> , 2005, , 1083-1092.	1.3	4
84	An innovative computational comparison of exact and centrifugal sudden quantum properties of the $\text{N} + \text{N} \langle \text{sub} \rangle 2 \langle /sub \rangle$ reaction. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 1589-1595.	2.8	4
85	A classical versus quantum mechanics study of the $\text{H} + \text{CO} \rightarrow \text{H} + \text{CO}_2$ ( $\text{J} = 0$ ) reaction. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	4
86	Closer versus Long Range Interaction Effects on the Non-Arrhenius Behavior of Quasi-Resonant $\text{O} \langle \text{sub} \rangle 2 \langle /sub \rangle + \text{N} \langle \text{sub} \rangle 2 \langle /sub \rangle$ Collisions. <i>Journal of Physical Chemistry A</i> , 2017, 121, 5088-5099.	2.5	4
87	Cooperative mechanisms for the $\text{H} + \text{ICl}$ reaction and their significance for the $\text{K} + \text{ICl}$ experiment. <i>Canadian Journal of Chemistry</i> , 1994, 72, 919-927.	1.1	3
88	Bond Order Potentials for a priori Simulations of Polyatomic Reactions. <i>Lecture Notes in Computer Science</i> , 2004, , 328-337.	1.3	3
89	Capture and dissociation in the complex-forming $\text{CH}(v = 0,1) + \text{D}_2 \hat{\text{t}}' \text{CHD} + \text{D}$ , $\text{CD}_2 + \text{H}$ , $\text{CD} + \text{HD}$ reactions and comparison with $\text{CH}(v = 0,1) + \text{H}_2$ . <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13638.	2.8	2
90	Collisional $\text{O}_2 + \text{N}_2$ State-Selected Cross Sections for Open Science Cloud Reuse. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6445-6457.	2.5	2

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91	Quasiclassical Calculations for Alkali and Alkaline Earth + Hydrogen Halide Chemical Reactions Using Supercomputers. , 1989, , 383-393.		2
92	Franck-Condon factors and R-centroids for the $A1\hat{\sim}+X1\hat{\sim}+$ and $B3\hat{\sim}(0+)\hat{\sim}X1\hat{\sim}+$ band system of $63\text{Cu}1\text{H}$ and $63\text{Cu}2\text{H}$ . Journal of Quantitative Spectroscopy and Radiative Transfer, 1983, 30, 439-447.	2.3	1
93	Temperature dependence of quasiclassical and quantum rate coefficients for $\text{N} + \text{N}_2$ . , 1994, , .		1
94	Temperature dependence of the rate coefficient of formation of CN radical from $\text{C}\hat{\sim}+\hat{\sim}\text{NH}$ . Chemical Physics Letters, 2021, 771, 138493.	2.6	1
95	A Quasiclassical Trajectory Study of Atom Diatom Reactions. Lecture Notes in Quantum Chemistry II, 2000, , 242-256.	0.3	0