TomÃ¡s GonzÃ¡lez-Lezana

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7186144/publications.pdf

Version: 2024-02-01

124 papers	2,840 citations	172457 29 h-index	214800 47 g-index
127 all docs	127 docs citations	127 times ranked	1123 citing authors

#	Article	IF	Citations
1	A rigorous test of the statistical model for atomâ€“diatom insertion reactions. Journal of Chemical Physics, 2003, 119, 12895-12907.	3.0	223
2	Statistical quantum studies on insertion atomâ€“diatom reactions. International Reviews in Physical Chemistry, 2007, 26, 29-91.	2.3	104
3	Experimental and Theoretical Differential Cross Sections for the N(2D) + H2Reactionâ€. Journal of Physical Chemistry A, 2006, 110, 817-829.	2.5	95
4	Quantum reactive scattering with a transmission-free absorbing potential. Journal of Chemical Physics, 2004, 120, 2247-2254.	3.0	93
5	Differential Cross Sections and Product Rotational Polarization in A + BC Reactions Using Wave Packet Methods: H⁺ + D₂ and Li + HF Examples. Journal of Physical Chemistry A, 2009, 113, 14488-14501.	2.5	86
6	Comparative configurational study for He, Ne, and Ar trimers. Journal of Chemical Physics, 1999, 110, 9000-9010.	3.0	70
7	A detailed quantum mechanical and quasiclassical trajectory study on the dynamics of the H++H2â†'H2+H+ exchange reaction. Journal of Chemical Physics, 2006, 125, 094314.	3.0	70
8	Efimov States forH4eTrimers?. Physical Review Letters, 1999, 82, 1648-1651.	7.8	69
9	Dynamics of the C(D1)+D2 reaction: A comparison of crossed molecular-beam experiments with quasiclassical trajectory and accurate statistical calculations. Journal of Chemical Physics, 2005, 122, 234309.	3.0	66
10	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>O</mml:mi><mml:mi>r</mml:mi><mml:mi>t</mml:mi><mml:mi>h</mml:mi><mml:mi>o</mml:mi><mml:mt mathvariant="normal">â^'</mml:mtext><mml:mi>P</mml:mi><mml:mi>a</mml:mi><mml:mi>r</mml:mi><mml:mi>a</mml:mi></mml:m xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Conversion by Proton Exchange at Low Temperature: An Accu. Physical Review Letters, 2011, 107, 023201.	7.8	62
11	Quantum approaches for the insertion dynamics of the H++D2 and D++H2 reactive collisions. Journal of Chemical Physics, 2005, 123, 194309.	3.0	61
12	Ortho-H₂and the age of prestellar cores. Astronomy and Astrophysics, 2013, 551, A38.	5.1	59
13	A statistical quasiclassical trajectory model for atom-diatom insertion reactions. Journal of Chemical Physics, 2007, 126, 161101.	3.0	58
14	On the dynamics of the H++D2(v=0,j=0)â†'HD+D+ reaction: A comparison between theory and experiment. Journal of Chemical Physics, 2008, 128, 014304.	3.0	57
15	A comparison of quantum and quasiclassical statistical models for reactions of electronically excited atoms with molecular hydrogen. Journal of Chemical Physics, 2008, 129, 094305.	3.0	51
16	Influence of rotation and isotope effects on the dynamics of the N(2D)+H2 reactive system and of its deuterated variants. Journal of Chemical Physics, 2005, 123, 224301.	3.0	47
17	Quasiclassical determination of reaction probabilities as a function of the total angular momentum. Journal of Chemical Physics, 2005, 123, 094101.	3.0	47
18	Vibrational predissociation dynamics of the He79Br2van der Waals molecule: A quantum mechanical study. Journal of Chemical Physics, 1996, 105, 7454-7463.	3.0	46

#	Article	IF	Citations
19	On the statistical behavior of the O+OHâ†'H+O2 reaction: A comparison between quasiclassical trajectory, quantum scattering, and statistical calculations. Journal of Chemical Physics, 2009, 130, 184301.	3.0	45
20	Stringent test of the statistical quasiclassical trajectory model for the H3+ exchange reaction: A comparison with rigorous statistical quantum mechanical results. Journal of Chemical Physics, 2007, 127, 174109.	3.0	44
21	The weakly bound ground state of the LiHe2 triatomic system. Physical Chemistry Chemical Physics, 2000, 2, 4067-4073.	2.8	41
22	Experimental and theoretical studies of the near-infrared spectrum of bromomethylene. Journal of Chemical Physics, 2001, 115, 5433-5444.	3.0	39
23	Solvation of ions in helium. International Reviews in Physical Chemistry, 2020, 39, 465-516.	2.3	38
24	A combined experimental-theoretical study of the vibrational predissociation and product rotational distributions for high vibrational levels of He79Br2. Journal of Chemical Physics, 1999, 110, 256-266.	3.0	35
25	Time dependent wave packet and statistical calculations on the H + O2reaction. Physical Chemistry Chemical Physics, 2007, 9, 1127-1137.	2.8	35
26	Study of the H+O2 reaction by means of quantum mechanical and statistical approaches: The dynamics on two different potential energy surfaces. Journal of Chemical Physics, 2008, 128, 244308.	3.0	32
27	Searching for Efimov states in triatomic systems: The case of LiHe 2. Europhysics Letters, 2000, 50, 567-573.	2.0	30
28	Parity conservation and polarization of differential cross sections in complex-forming chemical reactions. Physical Chemistry Chemical Physics, 2006, 8, 3951-3954.	2.8	30
29	Effects of the rotational excitation of D2 and of the potential energy surface on the H++D2â†'HD+D+ reaction. Journal of Chemical Physics, 2009, 131, 044315.	3.0	29
30	Ultracold chemistry with alkali-metalâ€“rare-earth molecules. Physical Review A, 2015, 91, .	2.5	29
31	Coronene molecules in helium clusters: Quantum and classical studies of energies and configurations. Journal of Chemical Physics, 2015, 143, 224306.	3.0	28
32	Dynamics of the D+ + H2 â†' HD + H+ reaction at the low energy regime by means of a statistical quantum method. Journal of Chemical Physics, 2013, 139, 054301.	3.0	26
33	Theoretical simulations of the He79Br2â€ŠB, v=8â†✗, vâ€³=0 excitation spectrum: Spectroscopic manifestation of a linear isomer?. Journal of Chemical Physics, 2000, 113, 4620-4628.	3.0	25
34	Lithium ions solvated in helium. Physical Chemistry Chemical Physics, 2018, 20, 25569-25576.	2.8	25
35	The H^{+â€‰}+â€‰H₂reaction. International Reviews in Physical Chemistry, 2014, 33, 371-395.	2.3	24
36	Ground states of weakly bound three-atom systems: energies and shapes of 4He2X clusters from Monte Carlo calculations. Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, 2643-2660.	1.5	23

#	Article	IF	Citations
37	Bound-state energies in argon trimers via a variational expansion: The effects from many-body corrections. Journal of Chemical Physics, 2005, 122, 144319.	3.0	23
38	Vibrational and rotational bound states in floppy triatomic systems: The distributed Gaussian functions approach. Physics Reports, 2007, 452, 1-32.	25.6	22
39	Nonadiabatic State-to-State Reactive Collisions among Open Shell Reactants with Conical Intersections: The OH(²Î) + F(²P) Example. Journal of Physical Chemistry A, 2010, 114, 9733-9742.	2.5	22
40	Quantum mechanical study of the proton exchange in the orthoâ€“para H2 conversion reaction at low temperature. Physical Chemistry Chemical Physics, 2011, 13, 19089.	2.8	22
41	Path integral Monte Carlo investigations on doped helium clusters. International Reviews in Physical Chemistry, 2016, 35, 37-68.	2.3	22
42	Adsorption of molecular hydrogen on coronene with a new potential energy surface. Physical Chemistry Chemical Physics, 2017, 19, 26358-26368.	2.8	22
43	Formation of rubidium dimers on the surface of helium clusters: a first step through quantum molecular dynamics simulations. European Physical Journal D, 2018, 72, 1.	1.3	22
44	Strongly mixed resonances in the photofragmentation of HeBr2 near Br2(B) dissociation: Stabilization and close-coupling studies. Journal of Chemical Physics, 1997, 106, 3216-3226.	3.0	21
45	A complete configurational study for the bound states of Ne trimers. Journal of Chemical Physics, 2005, 122, 084313.	3.0	21
46	A comparative study of the Si+O2â†'SiO+O reaction dynamics from quasiclassical trajectory and statistical based methods. Journal of Chemical Physics, 2008, 128, 174307.	3.0	21
47	A combined theoretical and experimental investigation of the kinetics and dynamics of the O(¹D) + D₂ reaction at low temperature. Physical Chemistry Chemical Physics, 2018, 20, 4404-4414.	2.8	21
48	The binding of He4 and He3 to a hydrogen molecule: A computational study for pH2 and oH2. Journal of Chemical Physics, 2005, 122, 084308.	3.0	20
49	The D⁺ + H₂ Reaction: Differential and Integral Cross Sections at Low Energy and Rate Constants at Low Temperature. Journal of Physical Chemistry A, 2014, 118, 6416-6424.	2.5	20
50	The dynamics of the C(1D)+H2/D2/HD reactions at low temperature. Journal of Chemical Physics, 2018, 148, 234305.	3.0	20
51	A variational method to treat diffuse states in weakly bound trimers. Computer Physics Communications, 2002, 145, 156-183.	7.5	19
52	Quantum Features of a Barely Bound Molecular Dopant: Cs₂(³Î£_u) in Bosonic Helium Droplets of Variable Size. Journal of Physical Chemistry A, 2011, 115, 6892-6902.	2.5	19
53	Spin-Polarized Rb₂ Interacting with Bosonic He Atoms: Potential Energy Surface and Quantum Structures of Small Clusters. Journal of Physical Chemistry A, 2012, 116, 2394-2404.	2.5	19
54	The structure of a weakly bound ionic trimer: Calculations for the 4He2Hâ^' complex. Journal of Chemical Physics, 2001, 114, 5520-5530.	3.0	18

#	Article	IF	Citations
55	A theoretical investigation on the spectrum of the Ar trimer for high rotational excitations. Journal of Chemical Physics, 2009, 130, 154301.	3.0	18
56	Wave packet and statistical quantum calculations for the He + NeH+ â†' HeH+ + Ne reaction on the ground electronic state. Journal of Chemical Physics, 2014, 141, 114302.	3.0	18
57	Scattering study of the Ne + NeH+(v = 0, j = 0) â†' NeH+ + Ne reaction on an ab initio based analytical potential energy surface. Journal of Chemical Physics, 2016, 144, 034303.	3.0	18
58	A combined experimental and theoretical investigation of Cs+ ions solvated in HeN clusters. Journal of Chemical Physics, 2019, 150, 154304.	3.0	17
59	Examination of the Feynmanâ€"Hibbs Approach in the Study of Ne_N-Coronene Clusters at Low Temperatures. Journal of Physical Chemistry A, 2016, 120, 5370-5379.	2.5	16
60	Comparative investigation of pure and mixed rare gas atoms on coronene molecules. Journal of Chemical Physics, 2017, 146, 034302.	3.0	16
61	A path-integral Monte Carlo study of a small cluster: The Ar trimer. Journal of Chemical Physics, 2010, 132, 244303.	3.0	15
62	H ₂ , H ₃ ⁺ and the age of molecular clouds and prestellar cores. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2012, 370, 5200-5212.	3.4	15
63	State-to-State Dynamics of the Ne + HeH⁺ (v = 0, j = 0) â†' NeH⁺(vâ€², jâ€²) + He Reaction. Journal of Physical Chemistry A, 2016, 120, 4731-4741.	2.5	15
64	Blueshifts of the Bâ†X excitation spectra of He79Br2 using a DIM-based potential. Chemical Physics Letters, 2000, 318, 578-584.	2.6	14
65	The Dynamics of the O(1D) + HCl â†' OH + Cl Reaction at a 0.26 eV Collision Energy: A Comparison between Theory and Experiment. Journal of Physical Chemistry A, 2009, 113, 14237-14250.	2.5	14
66	Energy dependent dynamics of the O(1D) + HCl reaction: A quantum, quasiclassical and statistical study. Physical Chemistry Chemical Physics, 2011, 13, 8502.	2.8	13
67	Snowball formation for Cs⁺ solvation in molecular hydrogen and deuterium. Physical Chemistry Chemical Physics, 2019, 21, 15662-15668.	2.8	12
68	Experimental and Theoretical Study of the O(¹D) + HD Reaction. Journal of Physical Chemistry A, 2019, 123, 8089-8098.	2.5	12
69	The O(1D) + H2 (Xâ€‰1Î£+, v, j) â†' OH(Xâ€‰2Î, vâ€², jâ€²) + H(2S) reaction at low collision energy: when a simple statistical description of the dynamics works. Physical Chemistry Chemical Physics, 2011, 13, 8136.	2.8	11
70	Rotationâ€"vibration interaction in 4He trimers. Chemical Physics Letters, 2001, 335, 105-110.	2.6	10
71	Helium aggregates doped with alkali dimer impurities: A finite temperature study of complexes. Computational and Theoretical Chemistry, 2012, 990, 106-111.	2.5	10
72	Quantum rotation of Rb2 (3 Î£ u +) attached to HeN droplets: a path-integral Monte Carlo study. European Physical Journal D, 2013, 67, 1.	1.3	10

#	Article	IF	Citations
73	Can the LiH molecule bind He atoms? A computational experiment. Chemical Physics Letters, 1999, 311, 255-264.	2.6	9
74	Symmetry assignment in the distributed Gaussian functions method to study homonuclear rotating trimers. Chemical Physics Letters, 2008, 460, 417-422.	2.6	9
75	Binding energies and structures of Ca-He<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>weakly bound triatomic complexes. Physical Review A, 2012, 86, .	2.5	9
76	Investigating transition state resonances in the time domain by means of Bohmian mechanics: The F+HD reaction. Chemical Physics, 2012, 399, 151-161.	1.9	9
77	Quantum, Statistical, and Quasiclassical Trajectory Studies For the Ne + HeH⁺ â†' NeH⁺ + He Reaction on the Ground Electronic State. Journal of Physical Chemistry A, 2015, 119, 12052-12061.	2.5	9
78	Half- and full-collision VT energy transfer in the Heî—¸Br2(B) system. Chemical Physics Letters, 1997, 269, 448-454.	2.6	8
79	Rovibrational Structures in Floppy Triatomics:Â Distributed Gaussian Functions Treatment for the Ne2H-Systemâ€. Journal of Physical Chemistry A, 2006, 110, 5487-5494.	2.5	8
80	An accurate study of the dynamics of the C+OH reaction on the second excited 14Aâ€³ potential energy surface. Journal of Chemical Physics, 2012, 136, 164309.	3.0	8
81	Binding weakly interacting partners: a study of Caâ€“He2 and its isotopomers. European Physical Journal D, 2012, 66, 1.	1.3	8
82	A configurational study of helium clusters doped with Heâ^—â^' and He2â^—â^'. Journal of Chemical Physics, 2015, 142, 104303.	3.0	8
83	Reactive scattering calculations for 87Rb+87RbHeâ†'Rb2(3Î£u+,v)+He from ultralow to intermediate energies. Journal of Chemical Physics, 2015, 142, 164304.	3.0	8
84	Rate constants for the H+ + H2 reaction from 5 K to 3000 K with a statistical quantum method. Journal of Chemical Physics, 2021, 154, 054310.	3.0	8
85	Dynamics of H + HeH⁺(v = 0, j = 0) â†' H₂⁺ + He: Insight on the Possible Complex-Forming Behavior of the Reaction. Journal of Physical Chemistry A, 2019, 123, 10480-10489.	2.5	7
86	Experimental and theoretical studies of the N(²D) + H₂ and D₂ reactions. Physical Chemistry Chemical Physics, 2020, 22, 23609-23617.	2.8	7
87	Rotational-state-changing collisions between <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msubsup><mml:mi mathvariant="normal">N</mml:mi><mml:mn>2</mml:mn><mml:mo>+</mml:mo></mml:msubsup></mml:math> and Rb at low energies. Physical Review A, 2020, 101, .	2.5	7
88	Comment on â€œEfimov States forH4eTrimers?â€• Physical Review Letters, 2001, 86, 4189-4189.	7.8	6
89	Diffusion Monte Carlo description of Cs₂(³Î£_u)â€"(⁴He)_Nclusters: an example of weak dopantâ€"helium interaction. Physica Scripta, 2011, 84, 028107.	2.5	6
90	Rovibrational transitions of H ₂ by collision with H ⁺ at high temperature. Monthly Notices of the Royal Astronomical Society, 0, , stx192.	4.4	6

#	Article	IF	Citations
91	Ca+ Ions Solvated in Helium Clusters. Molecules, 2021, 26, 3642.	3.8	6
92	Effective resolvent applied to interacting resonances. European Physical Journal D, 2001, 15, 215-219.	1.3	5
93	Quantum Zeno effect: Quantum shuffling and Markovianity. Annals of Physics, 2012, 327, 1277-1289.	2.8	5
94	Quantum Features of Anionic Species He^{*â€“} and He₂^{*â€“} in Small He_N Clusters. Journal of Physical Chemistry A, 2015, 119, 11574-11582.	2.5	5
95	Complexes of Alkali Metal Cations and Molecular Hydrogen: Potential Energy Surfaces and Bound States. Journal of Physical Chemistry A, 2019, 123, 8397-8405.	2.5	5
96	Growth of rare gases on coronene. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	5
97	Helium structures around SF₅⁺ and SF₆⁺: novel intermolecular potential and mass spectrometry experiments. Physical Chemistry Chemical Physics, 2022, 24, 2004-2014.	2.8	5
98	An adiabatic model for rare gasâ€“halogen van der Waals complexes: application to HeBr2(B).. Computational and Theoretical Chemistry, 1998, 433, 107-111.	1.5	4
99	GonzÃ¡lez-Lezanaet al.Reply:. Physical Review Letters, 2001, 86, 4190-4190.	7.8	4
100	Weakly bound finite systems: (4He)Nâ€“Rb2(3Î£u), clustering structures from a quantum Monte Carlo approach. Journal of Physics Condensed Matter, 2012, 24, 104014.	1.8	4
101	Communication: Quantum Zeno-based control mechanism for molecular fragmentation. Journal of Chemical Physics, 2012, 136, 121101.	3.0	4
102	Quasiclassical Trajectory and Statistical Quantum Calculations for the C + OH â†' CO + H Reaction on the First Excited 1²Aâ€³ Potential Energy Surface. Journal of Physical Chemistry A, 2013, 117, 1872-1879.	2.5	4
103	Path integral Monte Carlo calculations of calciumâ€doped ⁴He clusters. International Journal of Quantum Chemistry, 2014, 114, 1318-1326.	2.0	4
104	Theoretical methods for the rotationâ€“vibration spectra of triatomic molecules: distributed Gaussian functions compared with hyperspherical coordinates. International Reviews in Physical Chemistry, 2018, 37, 329-361.	2.3	4
105	Collisional cooling of primordial and interstellar media by H2. Monthly Notices of the Royal Astronomical Society, 2021, 507, 3564-3571.	4.4	4
106	On the features of statistical behaviour of the O(3P)+HCl(v = 2, j = 1,6,9) â†' OH + Cl reaction. European Physical Journal D, 2008, 47, 181-189.	1.3	3
107	A Study of the Ar3 System at Low Temperature. Few-Body Systems, 2009, 45, 237-239.	1.5	3
108	Limitations of a Theoretical Method to Calculate the Rovibrational Spectrum of Trimers: H $$^+_3$$ 3 +. Few-Body Systems, 2018, 59, 1.	1.5	3

#	Article	IF	Citations
109	Symmetry analysis of trimers rovibrational spectra: the case of Ne3. European Physical Journal D, 2018, 72, 1.	1.3	3
110	N2+(2Î£g) and Rb(2S) in a hybrid trap: modeling ion losses from radiative association paths. Physical Chemistry Chemical Physics, 2019, 21, 8342-8351.	2.8	3
111	Statistical investigations of the S<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e250" altimg="si4.svg"><mml:mrow><mml:mo>(</mml:mo><mml:msup><mml:mrow) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 657 Tc (reaction in the quantum regime. Chemical Physics Letters, 2021, 763, 138228.	2.6	3
112	Application of the stabilization method to interacting resonances. European Physical Journal D, 2002, 20, 227-232.	1.3	2
113	Binding He atoms to hydrogen moieties: quantum features from ultraweak interactions. Molecular Physics, 2010, 108, 57-72.	1.7	2
114	Comment on â€œWeakly bound states of the He-He-Ca triatomic systemâ€• Physical Review A, 2012, 86, .	2.5	2
115	Atomâ€“Diatom Reactive Scattering Collisions in Protonated Rare Gas Systems. Molecules, 2021, 26, 4206.	3.8	2
116	The Dynamics of the S(1D)+H2/D2 Reactions at Low Temperature via Statistical Simulations. Quarks, 2020, 3, 9-16.	0.3	2
117	The kinetics of Xâ€‰+â€‰H₂ reactions (Xâ€‰=â€‰C(¹D), N(²D), O(¹D),) Tj ET International Reviews in Physical Chemistry, 2021, 40, 457-493.	2.3	2
118	Theoretical spectroscopy and dynamics of fragmentation of the He79Br2 complex. , 1997, , .		1
119	Temperature dependence of the energetics and structure for the Ar dimer and trimer. International Journal of Quantum Chemistry, 2011, 111, 472-479.	2.0	1
120	Capture approximations beyond a statistical quantum mechanical method for atom-diatom reactions. European Physical Journal D, 2016, 70, 1.	1.3	1
121	On the Differential Cross Sections in Complex-Forming Atomâ€“Diatom Reactive Collisions. Progress in Theoretical Chemistry and Physics, 2009, , 47-66.	0.2	1
122	Variational and Path Integral Monte Carlo calculations on Helium Clusters Doped with Metastable Anions He*- and He2*-. Journal of Physics: Conference Series, 2015, 635, 072009.	0.4	0
123	STRUCTURE AND DYNAMICS OF VAN DER WAALS COMPLEXES: FROM TRIATOMIC TO MEDIUM SIZE CLUSTERS. , 2006, , .		0
124	Potential energy surfaces and dynamics of He n Br2 van der Waals complexes. Progress in Theoretical Chemistry and Physics, 2007, , 193-202.	0.2	0