Diego Troya

List of Publications by Year in descending order

111 papers	4,351 citations	87723 38 h-index	118652 62 g-index
112 all docs	112 docs citations	112 times ranked	3738 citing authors

#	Article	IF	Citations
1	The role of vacancy defects and holes in the fracture of carbon nanotubes. Chemical Physics Letters, 2004, 390, 413-420.	1.2	338
2	Mechanics of defects in carbon nanotubes: Atomistic and multiscale simulations. Physical Review B, 2005, 71, .	1.1	238
3	In Situ Probes of Capture and Decomposition of Chemical Warfare Agent Simulants by Zr-Based Metal Organic Frameworks. Journal of the American Chemical Society, 2017, 139, 599-602.	6.6	169
4	Bottlebrush Polymer Synthesis by Ring-Opening Metathesis Polymerization: The Significance of the Anchor Group. Journal of the American Chemical Society, 2016, 138, 6998-7004.	6.6	156
5	How Solvent Modulates Hydroxyl Radical Reactivity in Hydrogen Atom Abstractions. Journal of the American Chemical Society, 2010, 132, 2907-2913.	6.6	140
6	Mechanism and Kinetics for Reaction of the Chemical Warfare Agent Simulant, DMMP(g), with Zirconium(IV) MOFs: An Ultrahigh-Vacuum and DFT Study. Journal of Physical Chemistry C, 2017, 121, 11261-11272.	1.5	120
7	A crossed molecular beams study of the O(3P)+H2 reaction: Comparison of excitation function with accurate quantum reactive scattering calculations. Journal of Chemical Physics, 2003, 118, 1585-1588.	1.2	111
8	A quasiclassical trajectory study of the reaction OH+COâ†'H+CO2. Journal of Chemical Physics, 2003, 119, 5848-5859.	1.2	92
9	Surface Catalyzed Oxidative Oligomerization of 17Î²-Estradiol by Fe³⁺-Saturated Montmorillonite. Environmental Science & Technology, 2015, 49, 956-964.	4.6	91
10	Heterogeneous chemistry and reaction dynamics of the atmospheric oxidants, O₃, NO₃, and OH, on organic surfaces. Chemical Society Reviews, 2016, 45, 3731-3746.	18.7	90
11	Carbon nanotube fracture â€“ differences between quantum mechanical mechanisms and those of empirical potentials. Chemical Physics Letters, 2003, 382, 133-141.	1.2	88
12	Theoretical studies of hyperthermal O(3P) collisions with hydrocarbon self-assembled monolayers. Journal of Chemical Physics, 2004, 120, 7696-7707.	1.2	85
13	Reaction Mechanism of Nerve-Agent Decomposition with Zr-Based Metal Organic Frameworks. Journal of Physical Chemistry C, 2016, 120, 29312-29323.	1.5	84
14	Five New Zinc Phosphite Structures:â€‰ Tertiary Building Blocks in the Construction of Hybrid Materials. Inorganic Chemistry, 2005, 44, 2719-2727.	1.9	75
15	Crossed beams and theoretical studies of the O(3P)+CH4â†'H+OCH3 reaction excitation function. Journal of Chemical Physics, 2004, 120, 731-739.	1.2	72
16	Theoretical Studies of the O(3P) + Methane Reactionâ€. Journal of Physical Chemistry A, 2003, 107, 10497-10506.	1.1	71
17	Quantum wave packet and quasiclassical trajectory studies of OH+CO: Influence of the reactant channel well on thermal rate constants. Journal of Chemical Physics, 2004, 120, 1231-1238.	1.2	71
18	A Reinterpretation of the Mechanism of the Simplest Reaction at an sp3-Hybridized Carbon Atom:â€‰ H + CD4 â†' CD3 + HD. Journal of the American Chemical Society, 2005, 127, 11898-11899.	6.6	67

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19	Infrared Spectra and Binding Energies of Chemical Warfare Nerve Agent Simulants on the Surface of Amorphous Silica. Journal of Physical Chemistry C, 2013, 117, 15685-15697.	1.5	66
20	Hyperthermal Reactions of O(3P) with Alkanes:â€‰ Observations of Novel Reaction Pathways in Crossed-Beams and Theoretical Studies. Journal of Physical Chemistry A, 2003, 107, 4583-4587.	1.1	64
21	Experimental and Theoretical Investigations of the Inelastic and Reactive Scattering Dynamics of O(3P) + D2Ââ€. Journal of Physical Chemistry A, 2006, 110, 1327-1341.	1.1	61
22	Benzene, Toluene, and Xylene Transport through UiO-66: Diffusion Rates, Energetics, and the Role of Hydrogen Bonding. Journal of Physical Chemistry C, 2018, 122, 16060-16069.	1.5	60
23	Hyperthermal chemistry in the gas phase and on surfaces: theoretical studies. International Reviews in Physical Chemistry, 2004, 23, 341-373.	0.9	58
24	Multi-walled carbon nanotubes experiencing electrical breakdown as gas sensors. Nanotechnology, 2004, 15, 1596-1602.	1.3	56
25	H + CD4 Abstraction Reaction Dynamics:â€‰ Product Energy Partitioning. Journal of Physical Chemistry A, 2006, 110, 3017-3027.	1.1	54
26	Quasiclassical Trajectory Study of the O(3P) + CH4â†' OH + CH3Reaction with a Specific Reaction Parameters Semiempirical Hamiltonian. Journal of Physical Chemistry A, 2005, 109, 3015-3023.	1.1	52
27	H + CD4Abstraction Reaction Dynamics:Â Excitation Function and Angular Distributionsâ€. Journal of Physical Chemistry A, 2006, 110, 677-686.	1.1	52
28	Characterization of Undercoordinated Zr Defect Sites in UiO-66 with Vibrational Spectroscopy of Adsorbed CO. Journal of Physical Chemistry C, 2018, 122, 14582-14589.	1.5	52
29	Theoretical Study of the Arâ‹¯, Krâ‹¯, and Xeâ‹¯CH4, â‹¯CF4Intermolecular Potential-Energy Surfaces. Journal of Physical Chemistry A, 2006, 110, 10834-10843.	1.1	51
30	Theoretical Studies of the O(3P) + Ethane Reaction. Journal of Physical Chemistry A, 2003, 107, 7161-7169.	1.1	47
31	Ab initiopotential energy surface, variational transition state theory, and quasiclassical trajectory studies of the F+CH4â†'HF+CH3 reaction. Journal of Chemical Physics, 2004, 120, 5181-5191.	1.2	46
32	Metalâ€“Organic Framework- and Polyoxometalate-Based Sorbents for the Uptake and Destruction of Chemical Warfare Agents. ACS Applied Materials & Interfaces, 2020, 12, 14641-14661.	4.0	46
33	Classical trajectory study of collisions of Ar with alkanethiolate self-assembled monolayers: Potential-energy surface effects on dynamics. Journal of Chemical Physics, 2005, 122, 214712.	1.2	44
34	Quasiclassical Trajectory and Transition State Theory Studies of the N(4S) + H2â†" NH(X3Î£-) + H Reaction. Journal of Physical Chemistry A, 2002, 106, 4125-4136.	1.1	43
35	Ab initioand direct quasiclassical-trajectory study of the F+CH4â†'HF+CH3 reaction. Journal of Chemical Physics, 2005, 123, 214305.	1.2	43
36	Ab initio and direct quasiclassical-trajectory study of the Cl+CH4â†'HCl+CH3 reaction. Journal of Chemical Physics, 2006, 124, 074313.	1.2	41

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37	Theoretical Study of the Effect of Surface Density on the Dynamics of Ar + Alkanethiolate Self-Assembled Monolayer Collisionsâ€. Journal of Physical Chemistry A, 2006, 110, 1319-1326.	1.1	41
38	Ab initio, kinetics, and dynamics study of Cl+CH4â†'HCl+CH3. Journal of Chemical Physics, 2002, 117, 5730-5741.	1.2	40
39	Variational transition state theory and quasiclassical trajectory studies of the H2+OHâ†'H+H2O reaction and some isotopic variants. Journal of Chemical Physics, 2001, 115, 1828-1842.	1.2	38
40	A quasiclassical trajectory study of reactivity and product energy disposal in H+H2O, H+D2O, and H+HOD. Journal of Chemical Physics, 2001, 114, 8397-8413.	1.2	38
41	Chemical Warfare Agent Surface Adsorption: Hydrogen Bonding of Sarin and Soman to Amorphous Silica. Journal of Physical Chemistry Letters, 2014, 5, 1393-1399.	2.1	36
42	Crossed beams and theoretical studies of the dynamics of hyperthermal collisions between Ar and ethane. Journal of Chemical Physics, 2004, 121, 11702-11714.	1.2	35
43	Hyperthermal Ar atom scattering from a C(0001) surface. Journal of Chemical Physics, 2008, 128, 224708.	1.2	34
44	Adsorption of Substituted Benzene Derivatives on Silica: Effects of Electron Withdrawing and Donating Groups. Journal of Physical Chemistry C, 2016, 120, 13024-13031.	1.5	34
45	Molecular-Level Insight into CO₂ Adsorption on the Zirconium-Based Metalâ€“Organic Framework, UiO-66: A Combined Spectroscopic and Computational Approach. Journal of Physical Chemistry C, 2019, 123, 13731-13738.	1.5	34
46	Collisions of Polar and Nonpolar Gases with Hydrogen Bonding and Hydrocarbon Self-Assembled Monolayers. Journal of Physical Chemistry C, 2008, 112, 17272-17280.	1.5	32
47	Adsorption of 2-Chloroethyl Ethyl Sulfide on Silica: Binding Mechanism and Energy of a Bifunctional Hydrogen-Bond Acceptor at the Gasâ€“Surface Interface. Journal of Physical Chemistry C, 2015, 119, 365-372.	1.5	32
48	Theoretical study of the dynamics of the H+CH4 and H+C2H6 reactions using a specific-reaction-parameter semiempirical Hamiltonian. Journal of Chemical Physics, 2008, 128, 194302.	1.2	31
49	Experimental and theoretical studies of the effect of mass on the dynamics of gas/organic-surface energy transfer. Journal of Chemical Physics, 2008, 128, 014713.	1.2	30
50	Quasiclassical Trajectory Study of Energy and Angular Distributions for the H + CO2â†' OH + CO Reactionâ€. Journal of Physical Chemistry B, 2002, 106, 8148-8160.	1.2	28
51	Direct-Dynamics Study of the F + CH₄, C₂H₆, C₃H₈, and i-C₄H₁₀ Reactions. Journal of Physical Chemistry A, 2009, 113, 4294-4304.	1.1	24
52	Atomic-Level Structural Dynamics of Polyoxoniobates during DMMP Decomposition. Scientific Reports, 2017, 7, 773.	1.6	24
53	A quasiclassical trajectory study of product energy and angular distributions for the OH+D2 reaction. Journal of Chemical Physics, 2001, 115, 5160-5169.	1.2	23
54	Barriers of Hydrogen Abstraction from Primary, Secondary, and Tertiary Alkane Sites by O(³P). Journal of Physical Chemistry A, 2007, 111, 10745-10753.	1.1	23

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55	Correlated Multimodal Approach Reveals Key Details of Nerve-Agent Decomposition by Single-Site Zr-Based Polyoxometalates. Journal of Physical Chemistry Letters, 2019, 10, 2295-2299.	2.1	23
56	Classical Trajectory Study of the Dynamics of the Reaction of Cl Atoms with Ethane. Journal of Physical Chemistry A, 2008, 112, 9387-9395.	1.1	22
57	Quasi-classical trajectory study of the dynamics of the Cl + CH4â† ' HCl + CH3 reaction. Physical Chemistry Chemical Physics, 2011, 13, 11438.	1.3	22
58	Theoretical Study of the Adsorption of Organophosphorous Compounds to Models of a Silica Surface. Journal of Physical Chemistry C, 2013, 117, 14625-14634.	1.5	22
59	Studying â€˜chattering collisionsâ€™ in the Cl+ethane reaction with classical trajectories. Chemical Physics Letters, 2007, 441, 171-175.	1.2	21
60	Experimental and theoretical study of CO collisions with CH3- and CF3-terminated self-assembled monolayers. Journal of Chemical Physics, 2009, 130, 084702.	1.2	21
61	Interfacial energy exchange and reaction dynamics in collisions of gases on model organic surfaces. Progress in Surface Science, 2012, 87, 221-252.	3.8	21
62	Multimodal Characterization of Materials and Decontamination Processes for Chemical Warfare Protection. ACS Applied Materials & Interfaces, 2020, 12, 14721-14738.	4.0	21
63	A theoretical study of the ozonolysis of C₆₀: primary ozonide formation, dissociation, and multiple ozone additions. Physical Chemistry Chemical Physics, 2014, 16, 5977-5986.	1.3	20
64	Theoretical Study of the Dynamics of Collisions Between HCl and Ï‰-Hydroxylated Alkanethiol Self-Assembled Monolayers. Journal of Physical Chemistry C, 2011, 115, 2273-2283.	1.5	19
65	A quasiclassical trajectory study of the H+HCNâ† 'H2+CN reaction dynamics. Journal of Chemical Physics, 2000, 113, 6253-6263.	1.2	18
66	Quasiclassical Trajectory Study of Energy Transfer and Collision-Induced Dissociation in Hyperthermal Ar + CH4 and Ar + CF4 Collisions. Journal of Physical Chemistry A, 2005, 109, 5814-5824.	1.1	18
67	Theoretical Study of the Dynamics of Ar Collisions with C2H6and C2F6at Hyperthermal Energy. Journal of Physical Chemistry A, 2007, 111, 3618-3632.	1.1	18
68	Reaction Mechanism of Nerve-Agent Hydrolysis with the Cs8Nb6O19 Lindqvist Hexaniobate Catalyst. Journal of Physical Chemistry C, 2016, 120, 16822-16830.	1.5	18
69	Impact of ambient gases on the mechanism of [Cs8Nb6O19]-promoted nerve-agent decomposition. Chemical Science, 2018, 9, 2147-2158.	3.7	18
70	Self-amplified depolymerization of oligo(thiourethanes) for the release of COS/H₂S. Polymer Chemistry, 2019, 10, 2991-2995.	1.9	18
71	The dynamics of the O(1D)+N2Oâ† 'NO+NO reaction revisited: a QCT study on model potential energy surfaces. Chemical Physics Letters, 1999, 300, 603-612.	1.2	17
72	A quasiclassical trajectory study of angular and internal state distributions in H+H2O and H+D2O at E=1.4 eV. Chemical Physics Letters, 2001, 343, 420-428.	1.2	17

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73	Theoretical study of the dynamics of F+alkanethiol self-assembled monolayer hydrogen-abstraction reactions. Journal of Chemical Physics, 2010, 132, 134307.	1.2	17
74	Dynamics of collisions of hydroxyl radicals with fluorinated self-assembled monolayers. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	17
75	Systematic investigation of the excited-state properties of anthracene-dicarboxylic acids. Journal of Photochemistry and Photobiology A: Chemistry, 2017, 337, 207-215.	2.0	17
76	Insights into CO2 adsorption and chemical fixation properties of VPI-100 metalâ€“organic frameworks. Journal of Materials Chemistry A, 2018, 6, 22195-22203.	5.2	17
77	Geometry and energetics of CO adsorption on hydroxylated UiO-66. Physical Chemistry Chemical Physics, 2019, 21, 5078-5085.	1.3	17
78	Semiconducting and Metallic [5,5] Fullertube Nanowires: Characterization of Pristine D_{5h}(1)-C₉₀ and D_{5d}(1)-C₁₀₀. Journal of the American Chemical Society, 2021, 143, 4593-4599.	6.6	17
79	Relating Geometric Nanoconfinement and Local Molecular Environment to Diffusion in Ionic Polymer Membranes. Macromolecules, 2020, 53, 3296-3305.	2.2	16
80	A Quasiclassical Trajectory Study of the Cl + HCN â†' HCl + CN Reaction Dynamics. Microscopic Reaction Mechanism of the H(Cl) + HCN â†' H2(HCl) + CN Reactionsâ€. Journal of Physical Chemistry A, 2001, 105, 2285-2297.	1.1	14
81	A QCT study of the cross-section, energy and angular distributions of the OH+D2â†'HOD+D reaction at ET=0.28 eV on the YZCL2 surface. Chemical Physics Letters, 2004, 399, 527-533.	1.2	14
82	Theoretical study of the dynamics of hyperthermal collisions of Ar with a fluorinated alkanethiolate self-assembled monolayer. Physical Chemistry Chemical Physics, 2008, 10, 5776.	1.3	14
83	Theoretical Study of the Stereodynamics of CO Collisions with CH₃- and CF₃-Terminated Alkanethiolate Self-Assembled Monolayers. Journal of Physical Chemistry A, 2009, 113, 4155-4167.	1.1	13
84	Molecular Simulations of the Structure and Dynamics of Water Confined between Alkanethiol Self-Assembled Monolayer Plates. Journal of Physical Chemistry B, 2011, 115, 4662-4670.	1.2	13
85	Gas-surface reactions of nitrate radicals with vinyl-terminated self-assembled monolayers. Physical Chemistry Chemical Physics, 2014, 16, 16659-16670.	1.3	13
86	Ab Initio and Dynamics Study of the O(³P) + NH₃ and O(³P) + N₂H₄ Reactions at Hyperthermal Collision Energies. Journal of Physical Chemistry A, 2009, 113, 13863-13870.	1.1	11
87	Reaction Probability and Infrared Detection of the Primary Ozonide in Collisions of O₃ with Surface-Bound C₆₀. Journal of Physical Chemistry Letters, 2012, 3, 3193-3198.	2.1	11
88	Properties and Improved Space Survivability of POSS (Polyhedral Oligomeric Silsesquioxane) Polyimides. Materials Research Society Symposia Proceedings, 2004, 851, 487.	0.1	10
89	Reactivity Consequences of Conformational Isomerism in 1-Propanol. Journal of Physical Chemistry A, 2019, 123, 1044-1050.	1.1	9
90	Key mechanistic details of paraoxon decomposition by polyoxometalates: Critical role of para-nitro substitution. Chemical Physics, 2019, 518, 30-37.	0.9	8

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91	Atomic resolution tracking of nerve-agent simulant decomposition and host metalâ€“organic framework response in real space. Communications Chemistry, 2021, 4, .	2.0	8
92	Theoretical study of the dynamics of H+alkane reactions. Chemical Physics Letters, 2009, 467, 243-248.	1.2	7
93	Chemical Dynamics Simulations of the Hydroxyl Radical Reaction with Ethene. Chinese Journal of Chemical Physics, 2013, 26, 765-773.	0.6	7
94	Conformational Analysis of nâ†'Ï€* Interactions in Collagen Triple Helix Models. Journal of Physical Chemistry B, 2019, 123, 496-503.	1.2	7
95	Ab Initio and Quasiclassical Trajectory Study of the O(³P) + 2-Propanol Hydrogen Abstraction Reaction. Journal of Physical Chemistry A, 2019, 123, 6911-6920.	1.1	6
96	Insight into Hydrogen Abstractions by Nitrate Radical: Structural, Solvent Effects, and Evidence for a Polar Transition State. Journal of Physical Chemistry A, 2021, 125, 5471-5480.	1.1	5
97	Aqueous-Phase Destruction of Nerve-Agent Simulants at Copper Single Atoms in UiO-66. Inorganic Chemistry, 2022, 61, 8585-8591.	1.9	5
98	Size dependent ion-exchange of large mixed-metal complexes into Nafion^{Â®} membranes. Polymer Chemistry, 2015, 6, 6870-6879.	1.9	4
99	High-Resolution Comonomer Sequencing of Blocky Brominated Syndiotactic Polystyrene Copolymers Using ¹³C NMR Spectroscopy and Computer Simulations. Macromolecules, 2020, 53, 9539-9552.	2.2	4
100	Reversible Dissociation for Effective Storage of Diborane Gas within the UiO-66-NH2 Metalâ€“Organic Framework. ACS Applied Materials & Interfaces, 2022, , .	4.0	4
101	QUASICLASSICAL TRAJECTORY STUDIES OF FOUR-ATOM REACTIONS. Advanced Series in Physical Chemistry, 2004, , 249-290.	1.5	3
102	Dynamics Studies of the O(3P) + Ch4, C2H6 and C3H8 Reactions. , 2004, , 329-348.		3
103	Prolonged Association between Water Molecules under Hydrophobic Nanoconfinement. Journal of Physical Chemistry B, 2021, 125, 13767-13777.	1.2	3
104	Multichannel dynamics in the OH+ n-butane reaction revealed by crossed-beam slice imaging and quasiclassical trajectory calculations. Journal of Chemical Physics, 2020, 153, 014302.	1.2	2
105	Outdoor dissolution and photodegradation of insensitive munitions formulations IMX-101 and IMX-104: Photolytic transformation pathway and mechanism study. Chemosphere, 2021, 280, 130672.	4.2	2
106	Tribute to George C. Schatz. Journal of Physical Chemistry A, 2009, 113, 3709-3710.	1.1	1
107	Bifurcated Dihydrogen Bonding in the Uptake of Gas-Phase Diborane on Silica. Journal of Physical Chemistry Letters, 2021, 12, 4987-4992.	2.1	1
108	THEORETICAL STUDY OF REACTIONS OF HYPERTHERMAL O(3P)WITH PERFLUORINATED HYDROCARBONS. , 2006, , 365-375.		1

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109	Conformational Analysis of Fluoro-, Chloro-, and Proteo-Alkene Glyâ€“Pro and Proâ€“Pro Isosteres to Mimic Collagen. Journal of Physical Chemistry B, 2022, 126, 217-228.	1.2	1
110	Hyperthermal Chemistry in the Gas Phase and on Surfaces: Theoretical Studies. ChemInform, 2005, 36, no.	0.1	0
111	Dynamics of collisions of hydroxyl radicals with fluorinated self-assembled monolayers. , 2012, , 79-90.		0