Saulo A Vazquez

List of Publications by Year
in descending order

106	1,865	279798	361022
papers	citations	23 h-index	35 g-index

108	108	108	1411
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	An automated method to find reaction mechanisms and solve the kinetics in organometallic catalysis. Chemical Science, 2017, 8, 3843-3851.	7.4	81
2	Implementation of a fast analytic ground state potential energy surface for the N(2D)+H2 reaction. Journal of Chemical Physics, 2003, 119, 3063-3070.	3.0	62
3	Semiempirical Hamiltonian for Simulation of Azobenzene Photochemistry. Journal of Physical Chemistry A, 2012, 116, 98-110.	2.5	62
4	Absolute Configuration of Secondary Alcohols by 1H NMR:â€‰ In Situ Complexation of Î±-Methoxyphenylacetic Acid Esters with Barium(II). Journal of Organic Chemistry, 2002, 67, 4579-4589.	3.2	61
5	tsscds2018: A code for automated discovery of chemical reaction mechanisms and solving the kinetics. Journal of Computational Chemistry, 2018, 39, 1922-1930.	3.3	56
6	Quasiclassical Trajectory Study of the F + CH4Reaction Dynamics on a Dual-Level Interpolated Potential Energy Surface. Journal of Physical Chemistry A, 2005, 109, 8459-8470.	2.5	55
7	Quasi-classical trajectory calculations on a fast analytic potential energy surface for the C(1D)+H2 reaction. Chemical Physics Letters, 2003, 374, 243-251.	2.6	51
8	Quasiclassical dynamics simulation of the collision-induced dissociation of Cr(CO)6+ with Xe. Journal of Chemical Physics, 2005, 123, 154311.	3.0	48
9	Dynamics of CO₂ Scattering off a Perfluorinated Self-Assembled Monolayer. Influence of the Incident Collision Energy, Mass Effects, and Use of Different Surface Models. Journal of Physical Chemistry A, 2009, 113, 3850-3865.	2.5	45
10	Trajectory Dynamics Study of the Ar + CH4Dissociation Reaction at High Temperatures:Â the Importance of Zero-Point-Energy Effects. Journal of Physical Chemistry A, 2005, 109, 5415-5423.	2.5	44
11	<scp>AutoMeKin2021</scp>: An openâ€source program for automated reaction discovery. Journal of Computational Chemistry, 2021, 42, 2036-2048.	3.3	42
12	Role of Barium(II) in the Determination of the Absolute Configuration of Chiral Amines by1H NMR Spectroscopy. Journal of Organic Chemistry, 2006, 71, 1119-1130.	3.2	39
13	Influence of Multiple Conformations and Paths on Rate Constants and Product Branching Ratios. Thermal Decomposition of 1-Propanol Radicals. Journal of Physical Chemistry A, 2018, 122, 4790-4800.	2.5	37
14	The Role of Aromaticity in the Planarity of Lumiflavin. Journal of Organic Chemistry, 2002, 67, 6347-6352.	3.2	34
15	A Trajectory-Based Method to Explore Reaction Mechanisms. Molecules, 2018, 23, 3156.	3.8	33
16	Inelastic Scattering Dynamics of Ar from a Perfluorinated Self-Assembled Monolayer Surface. Journal of Physical Chemistry A, 2007, 111, 12785-12794.	2.5	32
17	Interaction and Dimerization Energies in Methyl-Blocked Î±,Î³-Peptide Nanotube Segments. Journal of Physical Chemistry B, 2010, 114, 4973-4983.	2.6	32
18	Hydrogen Transfer vs Proton Transfer in 7-Hydroxy-quinolineÂ·(NH3)3:Â A CASSCF/CASPT2 Study. Journal of Physical Chemistry A, 2007, 111, 5907-5912.	2.5	29

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19	HCN elimination from vinyl cyanide: product energy partitioning, the role of hydrogenâ€“deuterium exchange reactions and a new pathway. Physical Chemistry Chemical Physics, 2015, 17, 6948-6955.	2.8	28
20	Quasiclassical trajectory study of the collision-induced dissociation of CH[sub 3]SH[sup +]+Ar. Journal of Chemical Physics, 2004, 121, 2571.	3.0	26
21	Ab Initio and RRKM Study of the HCN/HNC Elimination Channels from Vinyl Cyanide. Journal of Physical Chemistry A, 2011, 115, 979-985.	2.5	26
22	Ab initio-gradient optimized molecular geometry and conformational analysis of 1,3-propanediol at the 4-21G level. Computational and Theoretical Chemistry, 1988, 181, 149-167.	1.5	25
23	Further investigation of the HCl elimination in the photodissociation of vinyl chloride at 193 nm: a direct MP2/6-31G(d,p) trajectory study. Chemical Physics Letters, 2004, 386, 225-232.	2.6	24
24	Collision-induced dissociation mechanisms of [Li(uracil)]+. Physical Chemistry Chemical Physics, 2013, 15, 7628.	2.8	24
25	A Direct Classical Trajectory Study of HCl Elimination from the 193 nm Photodissociation of Vinyl Chloride. Journal of Physical Chemistry A, 2003, 107, 7611-7618.	2.5	23
26	Dissociation of Difluoroethylenes. II. Direct Classical Trajectory Study of the HF Elimination from 1,2-Difluoroethylene. Journal of Physical Chemistry A, 2003, 107, 1398-1404.	2.5	23
27	Dynamics calculations for the Cl+C2H6 abstraction reaction: Thermal rate constants and kinetic isotope effects. Journal of Chemical Physics, 2003, 118, 6280-6288.	3.0	23
28	Direct and Indirect Hydrogen Abstraction in Cl + Alkene Reactions. Journal of Physical Chemistry A, 2014, 118, 5595-5607.	2.5	23
29	Recent applications of boxed molecular dynamics: a simple multiscale technique for atomistic simulations. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130384.	3.4	23
30	AB initio gradient optimized molecular geometry and conformational analysis of 1,2-propanediol at the 4-21G level. Computational and Theoretical Chemistry, 1989, 184, 323-342.	1.5	22
31	Three-center vs. four-center HF elimination from vinyl fluoride: a direct dynamics study. Chemical Physics Letters, 2000, 332, 583-590.	2.6	22
32	Quasiclassical Trajectory Study of the Collision-Induced Dissociation Dynamics of Ar + CH3SH+Using an Ab Initio Interpolated Potential Energy Surfaceâ€. Journal of Physical Chemistry A, 2006, 110, 1225-1231.	2.5	22
33	Product energy distributions for the four-center HF elimination from 1,1-difluoroethylene. A direct dynamics study. Chemical Physics Letters, 2001, 348, 81-88.	2.6	20
34	Photodissociation of formic acid: A trajectory surface hopping study. Chemical Physics Letters, 2005, 412, 35-40.	2.6	20
35	GAFit: A general-purpose, user-friendly program for fitting potential energy surfaces. Computer Physics Communications, 2017, 217, 89-98.	7.5	20
36	Unimolecular reaction dynamics of HSO. Analysis of the influence of different barrier samplings on the product energy distributions. Physical Chemistry Chemical Physics, 2002, 4, 279-287.	2.8	19

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37	Dissociation of Difluoroethylenes. I. Global Potential Energy Surface, RRKM, and VTST Calculations. Journal of Physical Chemistry A, 2003, 107, 1389-1397.	2.5	18
38	On the Conformational Memory in the Photodissociation of Formic Acid. Journal of Physical Chemistry A, 2005, 109, 2836-2839.	2.5	18
39	Theoretical and computational studies of non-equilibrium and non-statistical dynamics in the gas phase, in the condensed phase and at interfaces. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20170035.	3.4	18
40	Is Photolytic Production a Viable Source of HCN and HNC in Astrophysical Environments? A Laboratory-based Feasibility Study of Methyl Cyanoformate. Astrophysical Journal, 2017, 849, 15.	4.5	18
41	Ab initio-gradient optimized molecular geometry and conformational analysis of 2-methoxyethanol at the 4-21G level. Computational and Theoretical Chemistry, 1989, 188, 95-104.	1.5	17
42	Nonstatistical effects in the unimolecular dissociation of the acetyl radical. Journal of Chemical Physics, 1999, 110, 11323-11334.	3.0	17
43	Dissociation of ethylene and several deuterated derivatives at 193 and 157 nm by direct classical trajectories. Chemical Physics Letters, 2002, 353, 418-425.	2.6	17
44	Intermolecular Potential for Binding of Protonated Peptide Ions with Perfluorinated Hydrocarbon Surfaces. Journal of Physical Chemistry B, 2014, 118, 5577-5588.	2.6	17
45	Ab Initio Calculations on the Vinyl Fluoride Fragmentation Reactions. Structural Chemistry, 2001, 12, 95-100.	2.0	16
46	New lead(II) complexes with N,S-ligands, including a lead pyrazolonate with unusual packing flexibility. Polyhedron, 2007, 26, 4228-4238.	2.2	16
47	Molecular mechanics study of conformational trends in simple alcohols and ethers. II. Intramolecular hydrogen bonding. Journal of Computational Chemistry, 1992, 13, 851-859.	3.3	14
48	Direct Dynamics Study of the Dissociation and Elimination Channels in the Thermal Decomposition of Methyl Nitrite. Journal of the American Chemical Society, 1998, 120, 7594-7601.	13.7	14
49	A direct classical trajectory study of the acetone photodissociation on the triplet surface. Journal of Chemical Physics, 2003, 119, 10618-10625.	3.0	14
50	Rovibrational distributions of HF in the photodissociation of vinyl fluoride at 193 nm: A direct MP2 quasiclassical trajectory study. Journal of Chemical Physics, 2004, 121, 5179-5182.	3.0	14
51	Direct-Dynamics VTST Study of the [1,7] Hydrogen Shift in 7-Methylocta-1,3(Z),5(Z)-triene. A Model System for the Hydrogen Transfer Reaction in Previtamin D3. Journal of Physical Chemistry A, 2007, 111, 719-725.	2.5	14
52	Classical Dynamics Study of the Unimolecular Decomposition of CH3SH+. Journal of Physical Chemistry A, 1999, 103, 9783-9793.	2.5	13
53	Direct dynamics study of the photodissociation of triplet propanal at threshold. Chemical Physics Letters, 2003, 381, 37-44.	2.6	13
54	Dynamical study of the dissociation and elimination channels in the decomposition of methyl nitrite. Journal of Chemical Physics, 1998, 109, 8907-8919.	3.0	12

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55	A direct DFT dynamics study of the photodissociation of triplet acetaldehyde. Chemical Physics Letters, 2003, 375, 591-597.	2.6	12
56	Chemical Dynamics Simulations of CO₂in the Ground and First Excited Bend States Colliding with a Perfluorinated Self-Assembled Monolayer. Journal of Physical Chemistry C, 2010, 114, 18455-18464.	3.1	12
57	Further studies of the methyl nitrite cisâ†'trans isomerization. Journal of Chemical Physics, 1997, 107, 5393-5405.	3.0	11
58	Further dynamical studies of the dissociation and elimination reactions of methyl nitrite. Journal of Chemical Physics, 1999, 111, 10501-10510.	3.0	11
59	Direct dynamics simulation of the methanethiol cation decomposition. Chemical Physics Letters, 2000, 324, 88-94.	2.6	11
60	Quasi-classical trajectory study of H2 elimination in the photodissociation of difluoroethylenes at 193 nm. Journal of Chemical Physics, 2003, 118, 6941-6945.	3.0	11
61	Chemical Dynamics Study of NO Scattering from a Perfluorinated Self-Assembled Monolayer. Journal of Physical Chemistry C, 2011, 115, 23817-23830.	3.1	11
62	An investigation of the three oxidation forms of lumiflavin. Journal of the Chemical Society Perkin Transactions II, 1992, , 889.	0.9	10
63	Theoretical investigations on the vibronic coupling between the electronic states S0 and S1 of formic acid including the photodissociation at 248nm. Chemical Physics Letters, 2005, 407, 166-170.	2.6	10
64	Photodissociation of acryloyl chloride at 193 nm: interpretation of the product energy distributions, and new elimination pathways. Physical Chemistry Chemical Physics, 2016, 18, 5019-5026.	2.8	10
65	Rotational effects in the unimolecular dissociation of the acetyl radical. Chemical Physics Letters, 2000, 316, 471-476.	2.6	9
66	RRKM and direct MP2/6-31G(d,p) quasiclassical trajectory study of the H2 elimination in the photodissociation of vinyl chloride at 193 nm. Chemical Physics Letters, 2004, 396, 442-447.	2.6	9
67	Molecular dynamics simulations for designing biomimetic pores based on internally functionalized self-assembling Î±,Î³-peptide nanotubes. Physical Chemistry Chemical Physics, 2015, 17, 28586-28601.	2.8	9
68	Ab initio gradient conformational analysis of polyazocyclohexanes:1,4-diazocyclohexane, 1,3-diazocyclohexane and 1,3,5-triazocyclohexane. Computational and Theoretical Chemistry, 1990, 205, 223-234.	1.5	8
69	Dynamics of the cisâ€"trans isomerization and Clâ€"O dissociation of chlorine nitrite. Classical trajectory and statistical calculations. Physical Chemistry Chemical Physics, 2000, 2, 5393-5399.	2.8	8
70	Rotational distributions of HBr in the photodissociation of vinyl bromide at 193nm: An investigation by direct quasiclassical trajectory calculations. Chemical Physics Letters, 2006, 425, 22-27.	2.6	8
71	Intermolecular potentials for simulations of collisions of SiNCS+ and (CH3)2SiNCS+ ions with fluorinated self-assembled monolayers. Chemical Physics, 2012, 399, 193-204.	1.9	8
72	Theoretical study of some nitriles: Intramolecular hydrogen bonds and anomeric effect. Journal of Computational Chemistry, 1992, 13, 722-729.	3.3	7

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73	Classical Trajectory Study of the Cisâ^'Trans Isomerization and Fâ^'O Dissociation of FONO. Journal of Physical Chemistry A, 1998, 102, 8708-8715.	2.5	7
74	Rate constants and kinetic isotope effects for Cl+CH4â†'ClH+CH3: a comparison between LSC-IVR and statistical theories. Chemical Physics Letters, 2002, 360, 59-64.	2.6	7
75	Quasiclassical trajectory calculations on the photodissociation of CF2CHCl at 193nm: Product energy distributions for the HF and HCl eliminations. Journal of Chemical Physics, 2005, 122, 104316.	3.0	7
76	Ab initio and RRKM study of the elimination of HF and HCl from chlorofluoroethylene. Chemical Physics Letters, 2007, 435, 176-181.	2.6	7
77	Internal energy of HCl upon photolysis of 2-chloropropene at 193 nm investigated with time-resolved Fourier-transform spectroscopy and quasiclassical trajectories. Journal of Chemical Physics, 2008, 129, 224301.	3.0	7
78	A molecular mechanics study of conformational trends in simple alcohols and ethers. Part I: Geometric trends. Journal of Computational Chemistry, 1991, 12, 872-879.	3.3	6
79	Conformational analysis of model compounds of vitamin D by theoretical calculations. Journal of Computational Chemistry, 1997, 18, 1647-1655.	3.3	6
80	Anharmonic Quasiclassical Barrier Samplings in Trajectory Calculations and Their Influence on the Computed Product Energy Distributions. Journal of Physical Chemistry A, 2001, 105, 4808-4813.	2.5	6
81	Rate constants and isotope effects for the CH3+H2â†'CH4+H reaction by an approximate semiclassical initial-value representation method. Chemical Physics Letters, 2001, 341, 351-357.	2.6	6
82	A direct dynamics study of the H2 elimination from 2,5-dihydrofuran. Journal of Chemical Physics, 2001, 115, 7872-7880.	3.0	6
83	Translational energy distributions in the photodissociation of fluorobenzene. Chemical Physics, 2008, 349, 219-225.	1.9	6
84	The relative position of Ï€â€“Ï€ interacting rings notably changes the nature of the substituent effect. Physical Chemistry Chemical Physics, 2020, 22, 12068-12081.	2.8	6
85	New Approach for Correcting Noncovalent Interactions in Semiempirical Quantum Mechanical Methods: The Importance of Multiple-Orientation Sampling. Journal of Chemical Theory and Computation, 2021, 17, 5556-5567.	5.3	6
86	An ab initio gradient study of ethylhydrazine. Computational and Theoretical Chemistry, 1990, 206, 49-66.	1.5	5
87	The unimolecular dissociation of the propionyl radical: A classical dynamics study. Journal of Chemical Physics, 2001, 114, 3546-3553.	3.0	5
88	A Theoretical Study of the Dynamics of the S +c-C3H Reaction. Journal of Physical Chemistry A, 2002, 106, 8811-8819.	2.5	5
89	Rate constants for the CH3Oâ€...+â€...NO â†' CH3ONO reaction by classical trajectory and canonical variational transition state theory calculations. Journal of Physical Organic Chemistry, 2002, 15, 123-129.	1.9	5
90	Improved United-Atom Models for Perfluorinated Self-Assembled Monolayers. Journal of Physical Chemistry C, 2009, 113, 3300-3312.	3.1	5

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91	Unraveling the Factors That Control Soft Landing of Small Silyl Ions on Fluorinated Self-Assembled Monolayers. Journal of Physical Chemistry C, 2014, 118, 10159-10169.	3.1	5
92	DinÃ¡mica de reacciones unimoleculares en fase gas: Desviaciones del comportamiento estadÃstico. Quimica Nova, 2002, 25, 579-588.	0.3	5
93	Complete structural analysis of cyclic polyhalogenated monoterpenes. A force field 2-dimensional NMR study. Journal of Organic Chemistry, 1986, 51, 4970-4973.	3.2	4
94	Unimolecular decomposition of CH3SH+: an ab initio and RRKM study. Computational and Theoretical Chemistry, 2000, 505, 109-116.	1.5	4
95	Product energy distributions from ethylene photodissociation at 193 nm: a DFT direct classical trajectory study. Chemical Physics Letters, 2003, 369, 1-7.	2.6	4
96	Back to the Coordination Modes of the Thiosemicarbazonate Chain: New Insights from Diorganolead(IV) and Lead(II) Derivatives of Isatin-3-thiosemicarbazone. European Journal of Inorganic Chemistry, 2010, 2010, 4992-5004.	2.0	4
97	Electrostatic penetration effects stand at the heart of aromatic Ï€ interactions. Physical Chemistry Chemical Physics, 2022, 24, 8979-8991.	2.8	4
98	A statistical study of the methyl nitrite isomerization reaction: inverse secondary isotope effects. Chemical Physics Letters, 1999, 310, 209-214.	2.6	3
99	Ab initio and RRKM calculations on the dissociation of the propionyl radical. Journal of Molecular Structure, 2000, 556, 123-129.	3.6	3
100	Trajectory Dynamics Study of Collision-Induced Dissociation of the Ar+CH4Reaction at Hyperthermal Conditions:Â Vibrational Excitation and Isotope Substitution. Journal of Physical Chemistry A, 2006, 110, 7113-7121.	2.5	2
101	Vibrational Energy Relaxation of Deuterium Fluoride in d-Dichloromethane: Insights from Different Potentials. Journal of Chemical Theory and Computation, 2021, 17, 1277-1289.	5.3	2
102	The PM6-FGC Method: Improved Corrections for Amines and Amides. Molecules, 2022, 27, 1678.	3.8	2
103	An ab initio gradient study of trimethylhydrazine. Computational and Theoretical Chemistry, 1989, 184, 311-322.	1.5	1
104	Study of the geometric trends and rotational constants of 1-fluoro-2-propanol and 2-fluoropropanol by Ab Initio calculations. Tetrahedron Computer Methodology, 1989, 2, 85-92.	0.2	1
105	A theoretical study of 1-amino-3-butene and 3-butene-1-thiol. Structural Chemistry, 1992, 3, 225-229.	2.0	1
106	Relevance of weak intermolecular forces on the supramolecular structure of free or DMSO solvated 5-(4-X-benzylidene)rhodanines (XÂ=ÂF, Cl, Br, I). Journal of Molecular Structure, 2016, 1120, 100-114.	3.6	1