Saulo A Vazquez

List of Publications by Year in Descending Order

103 papers	1,623 citations	22 h-index	32 g-index
108 ext. papers	1,747 ext. citations	3.3 avg, IF	4.49 L-index

#	Paper	IF	Citations
103	Vibrational Energy Relaxation of Deuterium Fluoride in -Dichloromethane: Insights from Different Potentials. *Journal of Chemical Theory and Computation*, **2021**, 17, 1277-1289	6.4	0
102	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	6.4	3
101	AutoMeKin2021: An open-source program for automated reaction discovery. *Journal of Computational Chemistry*, **2021**, 42, 2036-2048	3.5	7
100	The relative position of π-interacting rings notably changes the nature of the substituent effect. *Physical Chemistry Chemical Physics*, **2020**, 22, 12068-12081	3.6	0
99	A Trajectory-Based Method to Explore Reaction Mechanisms. *Molecules*, **2018**, 23,	4.8	24
98	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	2.8	27
97	An automated method to find reaction mechanisms and solve the kinetics in organometallic catalysis. *Chemical Science*, **2017**, 8, 3843-3851	9.4	66
96	GAFit: A general-purpose, user-friendly program for fitting potential energy surfaces. *Computer Physics Communications*, **2017**, 217, 89-98	4.2	14
95	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,	3	14
94	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	4.7	12
93	Photodissociation of acryloyl chloride at 193 nm: interpretation of the product energy distributions, and new elimination pathways. *Physical Chemistry Chemical Physics*, **2016**, 18, 5019-26	3.6	8
92	Relevance of weak intermolecular forces on the supramolecular structure of free or DMSO solvated 5-(4-X-benzylidene)rhodanines (X = F, Cl, Br, I). *Journal of Molecular Structure*, **2016**, 1120, 100-114	3.4	1
91	Molecular dynamics simulations for designing biomimetic pores based on internally functionalized self-assembling β-peptide nanotubes. *Physical Chemistry Chemical Physics*, **2015**, 17, 28586-601	3.6	9
90	HCN elimination from vinyl cyanide: product energy partitioning, the role of hydrogen-deuterium exchange reactions and a new pathway. *Physical Chemistry Chemical Physics*, **2015**, 17, 6948-55	3.6	21
89	Direct and indirect hydrogen abstraction in Cl + alkene reactions. *Journal of Physical Chemistry A*, **2014**, 118, 5595-607	2.8	21
88	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	3.8	5
87	Intermolecular potential for binding of protonated peptide ions with perfluorinated hydrocarbon surfaces. *Journal of Physical Chemistry B*, **2014**, 118, 5577-88	3.4	16

86	Recent applications of boxed molecular dynamics: a simple multiscale technique for atomistic simulations. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2014**, 372,	3	20
85	Collision-induced dissociation mechanisms of [Li(uracil)]+. *Physical Chemistry Chemical Physics*, **2013**, 15, 7628-37	3.6	21
84	Semiempirical Hamiltonian for simulation of azobenzene photochemistry. *Journal of Physical Chemistry A*, **2012**, 116, 98-110	2.8	50
83	Intermolecular potentials for simulations of collisions of SiNCS+ and (CH3)2SiNCS+ ions with fluorinated self-assembled monolayers. *Chemical Physics*, **2012**, 399, 193-204	2.3	7
82	Ab initio and RRKM study of the HCN/HNC elimination channels from vinyl cyanide. *Journal of Physical Chemistry A*, **2011**, 115, 979-85	2.8	22
81	Chemical Dynamics Study of NO Scattering from a Perfluorinated Self-Assembled Monolayer. *Journal of Physical Chemistry C*, **2011**, 115, 23817-23830	3.8	9
80	Interaction and dimerization energies in methyl-blocked alpha,gamma-peptide nanotube segments. *Journal of Physical Chemistry B*, **2010**, 114, 4973-83	3.4	31
79	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	3.8	12
78	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	2.3	4
77	Improved United-Atom Models for Perfluorinated Self-Assembled Monolayers. *Journal of Physical Chemistry C*, **2009**, 113, 3300-3312	3.8	5
76	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, 3850-65	2.8	42
75	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	3.9	7
74	Translational energy distributions in the photodissociation of fluorobenzene. *Chemical Physics*, **2008**, 349, 219-225	2.3	6
73	Inelastic scattering dynamics of Ar from a perfluorinated self-assembled monolayer surface. *Journal of Physical Chemistry A*, **2007**, 111, 12785-94	2.8	32
72	Hydrogen transfer vs proton transfer in 7-hydroxy-quinoline.(NH3)3: a CASSCF/CASPT2 study. *Journal of Physical Chemistry A*, **2007**, 111, 5907-12	2.8	25
71	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, 719-25	2.8	14
70	Ab initio and RRKM study of the elimination of HF and HCl from chlorofluoroethylene. *Chemical Physics Letters*, **2007**, 435, 176-181	2.5	7
69	New lead(II) complexes with N,S-ligands, including a lead pyrazolonate with unusual packing flexibility. *Polyhedron*, **2007**, 26, 4228-4238	2.7	16

68	Role of barium(II) in the determination of the absolute configuration of chiral amines by 1H NMR spectroscopy. *Journal of Organic Chemistry*, **2006**, 71, 1119-30	4.2	35
67	Quasiclassical trajectory study of the collision-induced dissociation dynamics of Ar + CH3SH+ using an ab initio interpolated potential energy surface. *Journal of Physical Chemistry A*, **2006**, 110, 1225-31	2.8	21
66	Trajectory dynamics study of collision-induced dissociation of the Ar + CH4 reaction at hyperthermal conditions: vibrational excitation and isotope substitution. *Journal of Physical Chemistry A*, **2006**, 110, 7113-21	2.8	2
65	Rotational distributions of HBr in the photodissociation of vinyl bromide at 193 nm: An investigation by direct quasiclassical trajectory calculations. *Chemical Physics Letters*, **2006**, 425, 22-27	2.5	8
64	On the conformational memory in the photodissociation of formic acid. *Journal of Physical Chemistry A*, **2005**, 109, 2836-9	2.8	18
63	Trajectory dynamics study of the Ar + CH4 dissociation reaction at high temperatures: the importance of zero-point-energy effects. *Journal of Physical Chemistry A*, **2005**, 109, 5415-23	2.8	42
62	Quasiclassical trajectory study of the F + CH4 reaction dynamics on a dual-level interpolated potential energy surface. *Journal of Physical Chemistry A*, **2005**, 109, 8459-70	2.8	51
61	Theoretical investigations on the vibronic coupling between the electronic states S0 and S1 of formic acid including the photodissociation at 248 nm. *Chemical Physics Letters*, **2005**, 407, 166-170	2.5	8
60	Photodissociation of formic acid: A trajectory surface hopping study. *Chemical Physics Letters*, **2005**, 412, 35-40	2.5	19
59	Quasiclassical trajectory calculations on the photodissociation of CF2CHCl at 193 nm: product energy distributions for the HF and HCl eliminations. *Journal of Chemical Physics*, **2005**, 122, 104316	3.9	7
58	Quasiclassical dynamics simulation of the collision-induced dissociation of Cr(CO)6 + with Xe. *Journal of Chemical Physics*, **2005**, 123, 154311	3.9	44
57	Quasiclassical trajectory study of the collision-induced dissociation of CH3SH+ + Ar. *Journal of Chemical Physics*, **2004**, 121, 2571-7	3.9	26
56	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, 5179-82	3.9	14
55	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	2.5	22
54	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	2.5	8
53	Direct dynamics study of the photodissociation of triplet propanal at threshold. *Chemical Physics Letters*, **2003**, 381, 37-44	2.5	12
52	Product energy distributions from ethylene photodissociation at 193 nm: a DFT direct classical trajectory study. *Chemical Physics Letters*, **2003**, 369, 1-7	2.5	4
51	Quasi-classical trajectory calculations on a fast analytic potential energy surface for the C(1D)+H2 reaction. *Chemical Physics Letters*, **2003**, 374, 243-251	2.5	47

50	A direct DFT dynamics study of the photodissociation of triplet acetaldehyde. *Chemical Physics Letters*, **2003**, 375, 591-597	2.5	12
49	Dissociation of Difluoroethylenes. I. Global Potential Energy Surface, RRKM, and VTST Calculations. *Journal of Physical Chemistry A*, **2003**, 107, 1389-1397	2.8	18
48	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	2.8	22
47	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	2.8	23
46	Dynamics calculations for the Cl+C2H6 abstraction reaction: Thermal rate constants and kinetic isotope effects. *Journal of Chemical Physics*, **2003**, 118, 6280-6288	3.9	21
45	Implementation of a fast analytic ground state potential energy surface for the N(2D)+H2 reaction. *Journal of Chemical Physics*, **2003**, 119, 3063-3070	3.9	59
44	Quasi-classical trajectory study of H2 elimination in the photodissociation of difluoroethylenes at 193 nm. *Journal of Chemical Physics*, **2003**, 118, 6941-6945	3.9	10
43	A direct classical trajectory study of the acetone photodissociation on the triplet surface. *Journal of Chemical Physics*, **2003**, 119, 10618-10625	3.9	12
42	Rate constants for the CH3O + NO -þCH3ONO reaction by classical trajectory and canonical variational transition state theory calculations. *Journal of Physical Organic Chemistry*, **2002**, 15, 123-129	2.1	4
41	Dissociation of ethylene and several deuterated derivatives at 193 and 157 nm by direct classical trajectories. *Chemical Physics Letters*, **2002**, 353, 418-425	2.5	15
40	Rate constants and kinetic isotope effects for Cl+CH4-þlH+CH3: a comparison between LSC-IVR and statistical theories. *Chemical Physics Letters*, **2002**, 360, 59-64	2.5	7
39	The role of aromaticity in the planarity of lumiflavin. *Journal of Organic Chemistry*, **2002**, 67, 6347-52	4.2	31
38	Absolute configuration of secondary alcohols by 1H NMR: in situ complexation of alpha-methoxyphenylacetic acid esters with barium(II). *Journal of Organic Chemistry*, **2002**, 67, 4579-89	4.2	57
37	A Theoretical Study of the Dynamics of the S + c-C3H Reaction. *Journal of Physical Chemistry A*, **2002**, 106, 8811-8819	2.8	4
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	3.6	18
35	Din□mica de reacciones unimoleculares en fase gas: Desviaciones del comportamiento estad□stico. *Quimica Nova*, **2002**, 25, 579-588	1.6	4
34	Rate constants and isotope effects for the CH3+H2-þH4+H reaction by an approximate semiclassical initial-value representation method. *Chemical Physics Letters*, **2001**, 341, 351-357	2.5	6
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	2.5	20

32	Ab Initio Calculations on the Vinyl Fluoride Fragmentation Reactions. *Structural Chemistry*, **2001**, 12, 95-108	1.8	16
31	A direct dynamics study of the H2 elimination from 2,5-dihydrofuran. *Journal of Chemical Physics*, **2001**, 115, 7872-7880	3.9	6
30	The unimolecular dissociation of the propionyl radical: A classical dynamics study. *Journal of Chemical Physics*, **2001**, 114, 3546-3553	3.9	4
29	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	2.8	5
28	Direct dynamics simulation of the methanethiol cation decomposition. *Chemical Physics Letters*, **2000**, 324, 88-94	2.5	9
27	Three-center vs. four-center HF elimination from vinyl fluoride: a direct dynamics study. *Chemical Physics Letters*, **2000**, 332, 583-590	2.5	20
26	Rotational effects in the unimolecular dissociation of the acetyl radical. *Chemical Physics Letters*, **2000**, 316, 471-476	2.5	6
25	Ab initio and RRKM calculations on the dissociation of the propionyl radical. *Journal of Molecular Structure*, **2000**, 556, 123-129	3.4	3
24	Unimolecular decomposition of CH3SH+: an ab initio and RRKM study. *Computational and Theoretical Chemistry*, **2000**, 505, 109-116		4
23	Dynamics of the cis□trans isomerization and ClO dissociation of chlorine nitrite. Classical trajectory and statistical calculations. *Physical Chemistry Chemical Physics*, **2000**, 2, 5393-5399	3.6	8
22	Further dynamical studies of the dissociation and elimination reactions of methyl nitrite. *Journal of Chemical Physics*, **1999**, 111, 10501-10510	3.9	9
21	A statistical study of the methyl nitrite isomerization reaction: inverse secondary isotope effects. *Chemical Physics Letters*, **1999**, 310, 209-214	2.5	2
20	Nonstatistical effects in the unimolecular dissociation of the acetyl radical. *Journal of Chemical Physics*, **1999**, 110, 11323-11334	3.9	15
19	Classical Dynamics Study of the Unimolecular Decomposition of CH3SH+. *Journal of Physical Chemistry A*, **1999**, 103, 9783-9793	2.8	11
18	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	16.4	14
17	Classical Trajectory Study of the Cis□trans Isomerization and FO Dissociation of FONO. *Journal of Physical Chemistry A*, **1998**, 102, 8708-8715	2.8	6
16	Dynamical study of the dissociation and elimination channels in the decomposition of methyl nitrite. *Journal of Chemical Physics*, **1998**, 109, 8907-8919	3.9	10
15	Further studies of the methyl nitrite cis-trans isomerization. *Journal of Chemical Physics*, **1997**, 107, 5393-5405	3.9	8

14	Conformational analysis of model compounds of vitamin D by theoretical calculations. *Journal of Computational Chemistry*, **1997**, 18, 1647-1655	3.5	4
13	An investigation of the three oxidation forms of lumiflavin. *Journal of the Chemical Society Perkin Transactions II*, **1992**, 889		9
12	A theoretical study of 1-amino-3-butene and 3-butene-1-thiol. *Structural Chemistry*, **1992**, 3, 225-229	1.8	1
11	Theoretical study of some nitriles: Intramolecular hydrogen bonds and anomeric effect. *Journal of Computational Chemistry*, **1992**, 13, 722-729	3.5	7
10	Molecular mechanics study of conformational trends in simple alcohols and ethers. II. Intramolecular hydrogen bonding. *Journal of Computational Chemistry*, **1992**, 13, 851-859	3.5	14
9	A molecular mechanics study of conformational trends in simple alcohols and ethers. Part I: Geometric trends. *Journal of Computational Chemistry*, **1991**, 12, 872-879	3.5	6
8	An ab initio gradient study of ethylhydrazine. *Computational and Theoretical Chemistry*, **1990**, 206, 49-66		4
7	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		7
6	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		15
5	An ab initio gradient study of trimethylhydrazine. *Computational and Theoretical Chemistry*, **1989**, 184, 311-322		1
4	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		22
3	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		1
2	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		22
1	Complete structural analysis of cyclic polyhalogenated monoterpenes. A force field 2-dimensional NMR study. *Journal of Organic Chemistry*, **1986**, 51, 4970-4973	4.2	3