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	Electrostatic penetration effects stand at the heart of aromatic Ï€ interactions. Physical Chemistry Chemical Physics, 2022, 24, 8979-8991.	2.8	4
2	The PM6-FGC Method: Improved Corrections for Amines and Amides. Molecules, 2022, 27, 1678.	3.8	2
3	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
4	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
5	<scp>AutoMeKin2021</scp>: An openâ€source program for automated reaction discovery. Journal of Computational Chemistry, 2021, 42, 2036-2048.	3.3	42
6	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
7	A Trajectory-Based Method to Explore Reaction Mechanisms. Molecules, 2018, 23, 3156.	3.8	33
8	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
9	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
10	An automated method to find reaction mechanisms and solve the kinetics in organometallic catalysis. Chemical Science, 2017, 8, 3843-3851.	7.4	81
11	GAFit: A general-purpose, user-friendly program for fitting potential energy surfaces. Computer Physics Communications, 2017, 217, 89-98.	7.5	20
12	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
13	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
14	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
15	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
16	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
17	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
18	Direct and Indirect Hydrogen Abstraction in Cl + Alkene Reactions. Journal of Physical Chemistry A, 2014, 118, 5595-5607.	2.5	23

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19	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
20	Intermolecular Potential for Binding of Protonated Peptide Ions with Perfluorinated Hydrocarbon Surfaces. Journal of Physical Chemistry B, 2014, 118, 5577-5588.	2.6	17
21	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
22	Collision-induced dissociation mechanisms of [Li(uracil)]+. Physical Chemistry Chemical Physics, 2013, 15, 7628.	2.8	24
23	Semiempirical Hamiltonian for Simulation of Azobenzene Photochemistry. Journal of Physical Chemistry A, 2012, 116, 98-110.	2.5	62
24	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
25	Chemical Dynamics Study of NO Scattering from a Perfluorinated Self-Assembled Monolayer. Journal of Physical Chemistry C, 2011, 115, 23817-23830.	3.1	11
26	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
27	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
28	Interaction and Dimerization Energies in Methyl-Blocked Î±,Î³-Peptide Nanotube Segments. Journal of Physical Chemistry B, 2010, 114, 4973-4983.	2.6	32
29	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
30	Improved United-Atom Models for Perfluorinated Self-Assembled Monolayers. Journal of Physical Chemistry C, 2009, 113, 3300-3312.	3.1	5
31	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
32	Translational energy distributions in the photodissociation of fluorobenzene. Chemical Physics, 2008, 349, 219-225.	1.9	6
33	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
34	Inelastic Scattering Dynamics of Ar from a Perfluorinated Self-Assembled Monolayer Surface. Journal of Physical Chemistry A, 2007, 111, 12785-12794.	2.5	32
35	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
36	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

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37	Ab initio and RRKM study of the elimination of HF and HCl from chlorofluoroethylene. Chemical Physics Letters, 2007, 435, 176-181.	2.6	7
38	New lead(II) complexes with N,S-ligands, including a lead pyrazolonate with unusual packing flexibility. Polyhedron, 2007, 26, 4228-4238.	2.2	16
39	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
40	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
41	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
42	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
43	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
44	Photodissociation of formic acid: A trajectory surface hopping study. Chemical Physics Letters, 2005, 412, 35-40.	2.6	20
45	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
46	Quasiclassical dynamics simulation of the collision-induced dissociation of Cr(CO)6+ with Xe. Journal of Chemical Physics, 2005, 123, 154311.	3.0	48
47	On the Conformational Memory in the Photodissociation of Formic Acid. Journal of Physical Chemistry A, 2005, 109, 2836-2839.	2.5	18
48	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
49	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
50	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
51	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
52	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
53	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
54	Direct dynamics study of the photodissociation of triplet propanal at threshold. Chemical Physics Letters, 2003, 381, 37-44.	2.6	13

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55	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
56	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
57	A direct DFT dynamics study of the photodissociation of triplet acetaldehyde. Chemical Physics Letters, 2003, 375, 591-597.	2.6	12
58	Dissociation of Difluoroethylenes. I. Global Potential Energy Surface, RRKM, and VTST Calculations. Journal of Physical Chemistry A, 2003, 107, 1389-1397.	2.5	18
59	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
60	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
61	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
62	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
63	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
64	A direct classical trajectory study of the acetone photodissociation on the triplet surface. Journal of Chemical Physics, 2003, 119, 10618-10625.	3.0	14
65	The Role of Aromaticity in the Planarity of Lumiflavin. Journal of Organic Chemistry, 2002, 67, 6347-6352.	3.2	34
66	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
67	A Theoretical Study of the Dynamics of the S +c-C3H Reaction. Journal of Physical Chemistry A, 2002, 106, 8811-8819.	2.5	5
68	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
69	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
70	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
71	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
72	DinÃ¡mica de reacciones unimoleculares en fase gas: Desviaciones del comportamiento estadÃstico. Quimica Nova, 2002, 25, 579-588.	0.3	5

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73	The unimolecular dissociation of the propionyl radical: A classical dynamics study. Journal of Chemical Physics, 2001, 114, 3546-3553.	3.0	5
74	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
75	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
76	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
77	Ab Initio Calculations on the Vinyl Fluoride Fragmentation Reactions. Structural Chemistry, 2001, 12, 95-100.	2.0	16
78	A direct dynamics study of the H2 elimination from 2,5-dihydrofuran. Journal of Chemical Physics, 2001, 115, 7872-7880.	3.0	6
79	Direct dynamics simulation of the methanethiol cation decomposition. Chemical Physics Letters, 2000, 324, 88-94.	2.6	11
80	Three-center vs. four-center HF elimination from vinyl fluoride: a direct dynamics study. Chemical Physics Letters, 2000, 332, 583-590.	2.6	22
81	Rotational effects in the unimolecular dissociation of the acetyl radical. Chemical Physics Letters, 2000, 316, 471-476.	2.6	9
82	Ab initio and RRKM calculations on the dissociation of the propionyl radical. Journal of Molecular Structure, 2000, 556, 123-129.	3.6	3
83	Unimolecular decomposition of CH3SH+: an ab initio and RRKM study. Computational and Theoretical Chemistry, 2000, 505, 109-116.	1.5	4
84	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
85	Further dynamical studies of the dissociation and elimination reactions of methyl nitrite. Journal of Chemical Physics, 1999, 111, 10501-10510.	3.0	11
86	A statistical study of the methyl nitrite isomerization reaction: inverse secondary isotope effects. Chemical Physics Letters, 1999, 310, 209-214.	2.6	3
87	Nonstatistical effects in the unimolecular dissociation of the acetyl radical. Journal of Chemical Physics, 1999, 110, 11323-11334.	3.0	17
88	Classical Dynamics Study of the Unimolecular Decomposition of CH3SH+. Journal of Physical Chemistry A, 1999, 103, 9783-9793.	2.5	13
89	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
90	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

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91	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
92	Further studies of the methyl nitrite cisâ†'trans isomerization. Journal of Chemical Physics, 1997, 107, 5393-5405.	3.0	11
93	Conformational analysis of model compounds of vitamin D by theoretical calculations. Journal of Computational Chemistry, 1997, 18, 1647-1655.	3.3	6
94	An investigation of the three oxidation forms of lumiflavin. Journal of the Chemical Society Perkin Transactions II, 1992, , 889.	0.9	10
95	A theoretical study of 1-amino-3-butene and 3-butene-1-thiol. Structural Chemistry, 1992, 3, 225-229.	2.0	1
96	Theoretical study of some nitriles: Intramolecular hydrogen bonds and anomeric effect. Journal of Computational Chemistry, 1992, 13, 722-729.	3.3	7
97	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
98	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
99	An ab initio gradient study of ethylhydrazine. Computational and Theoretical Chemistry, 1990, 206, 49-66.	1.5	5
100	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
101	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
102	An ab initio gradient study of trimethylhydrazine. Computational and Theoretical Chemistry, 1989, 184, 311-322.	1.5	1
103	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
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	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
106	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