Emilio Martinez-Nunez

List of Publications by Citations

129 papers	28,115 citations	28 h-index	137 g-index
137 ext. papers	29,393 ext. citations	3.6 avg, IF	7.66 L-index

#	Paper	IF	Citations
129	Development and use of quantum mechanical molecular models. 76. AM1: a new general purpose quantum mechanical molecular model. *Journal of the American Chemical Society*, **1985**, 107, 3902-3909	16.4	12010
128	Optimization of parameters for semiempirical methods I. Method. *Journal of Computational Chemistry*, **1989**, 10, 209-220	3.5	6553
127	Optimization of parameters for semiempirical methods V: modification of NDDO approximations and application to 70 elements. *Journal of Molecular Modeling*, **2007**, 13, 1173-213	2	2577
126	MOPAC: a semiempirical molecular orbital program. *Journal of Computer-Aided Molecular Design*, **1990**, 4, 1-105	4.2	2256
125	Optimization of parameters for semiempirical methods VI: more modifications to the NDDO approximations and re-optimization of parameters. *Journal of Molecular Modeling*, **2013**, 19, 1-32	2	1126
124	RM1: a reparameterization of AM1 for H, C, N, O, P, S, F, Cl, Br, and I. *Journal of Computational Chemistry*, **2006**, 27, 1101-11	3.5	571
123	Application of localized molecular orbitals to the solution of semiempirical self-consistent field equations. *International Journal of Quantum Chemistry*, **1996**, 58, 133-146	2.1	303
122	Application of the PM6 method to modeling proteins. *Journal of Molecular Modeling*, **2009**, 15, 765-805	2	235
121	Optimization of parameters for semiempirical methods IV: extension of MNDO, AM1, and PM3 to more main group elements. *Journal of Molecular Modeling*, **2004**, 10, 155-64	2	213
120	Application of the PM6 method to modeling the solid state. *Journal of Molecular Modeling*, **2008**, 14, 499-535	2	125
119	An automated method to find transition states using chemical dynamics simulations. *Journal of Computational Chemistry*, **2015**, 36, 222-34	3.5	111
118	Comparison of the accuracy of semiempirical and some DFT methods for predicting heats of formation. *Journal of Molecular Modeling*, **2004**, 10, 6-12	2	95
117	An automated transition state search using classical trajectories initialized at multiple minima. *Physical Chemistry Chemical Physics*, **2015**, 17, 14912-21	3.6	72
116	An automated method to find reaction mechanisms and solve the kinetics in organometallic catalysis. *Chemical Science*, **2017**, 8, 3843-3851	9.4	66
115	Chemical Dynamics Simulations of CO2Scattering off a Fluorinated Self-Assembled Monolayer Surface. *Journal of Physical Chemistry C*, **2007**, 111, 354-364	3.8	66
114	DFT conformational study of cysteine in gas phase and aqueous solution. *Computational and Theoretical Chemistry*, **2000**, 498, 191-200		60
113	Single-Valued DMBE Potential Energy Surface for HSO:´A Distributedn-Body Polynomial Approach. *Journal of Physical Chemistry A*, **2001**, 105, 5923-5932	2.8	60

112	Development and use of quantum mechanical molecular models. 76. AM1: a new general purpose quantum mechanical molecular model. [Erratum to document cited in CA103(2):11627f]. *Journal of the American Chemical Society*, **1993**, 115, 5348-5348	16.4	59
111	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
110	Semiempirical Hamiltonian for simulation of azobenzene photochemistry. *Journal of Physical Chemistry A*, **2012**, 116, 98-110	2.8	50
109	Quasiclassical dynamics simulation of the collision-induced dissociation of Cr(CO)6 + with Xe. *Journal of Chemical Physics*, **2005**, 123, 154311	3.9	44
108	Intermolecular interactions and cooperative effects in acetonitrile clusters. An ab initio molecular orbital study. *Computational and Theoretical Chemistry*, **2000**, 498, 21-28		43
107	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
106	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
105	Chemical Dynamics Simulations of Energy Transfer in Collisions of Protonated Peptide Ions with a Perfluorinated Alkylthiol Self-Assembled Monolayer Surface. *Journal of Physical Chemistry C*, **2008**, 112, 9377-9386	3.8	35
104	Inelastic scattering dynamics of Ar from a perfluorinated self-assembled monolayer surface. *Journal of Physical Chemistry A*, **2007**, 111, 12785-94	2.8	32
103	The role of aromaticity in the planarity of lumiflavin. *Journal of Organic Chemistry*, **2002**, 67, 6347-52	4.2	31
102	On the gas phase fragmentation of protonated uracil: a statistical perspective. *Physical Chemistry Chemical Physics*, **2016**, 18, 14980-90	3.6	28
101	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
100	Quasiclassical trajectory study of the collision-induced dissociation of CH3SH+ + Ar. *Journal of Chemical Physics*, **2004**, 121, 2571-7	3.9	26
99	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
98	Use of Semiempirical Methods for Detecting Anomalies in Reported Enthalpies of Formation of Organic Compounds. *Journal of Physical and Chemical Reference Data*, **2004**, 33, 713-724	4.3	24
97	A Trajectory-Based Method to Explore Reaction Mechanisms. *Molecules*, **2018**, 23,	4.8	24
96	Acceleration of Classical Mechanics by Phase Space Constraints. *Journal of Chemical Theory and Computation*, **2006**, 2, 912-9	6.4	23
95	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

94	An investigation into the applicability of the semiempirical method PM7 for modeling the catalytic mechanism in the enzyme chymotrypsin. *Journal of Molecular Modeling*, **2017**, 23, 154	2	22
93	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
92	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
91	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
90	Methanol dimer formation drastically enhances hydrogen abstraction from methanol by OH at low temperature. *Physical Chemistry Chemical Physics*, **2016**, 18, 22712-8	3.6	21
89	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
88	Collision-induced dissociation mechanisms of [Li(uracil)]+. *Physical Chemistry Chemical Physics*, **2013** , 15, 7628-37	3.6	21
87	Classical, quantum and statistical simulations of vibrationally excited HOSO(2): IVR, dissociation, and implications for OH + SO(2) kinetics at high pressures. *Physical Chemistry Chemical Physics*, **2009** , 11, 963-74	3.6	21
86	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
85	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
84	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
83	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
82	Three-center vs. four-center HF elimination from vinyl fluoride: a direct dynamics study. *Chemical Physics Letters*, **2000**, 332, 583-590	2.5	20
81	Photodissociation of formic acid: A trajectory surface hopping study. *Chemical Physics Letters*, **2005**, 412, 35-40	2.5	19
80	On the conformational memory in the photodissociation of formic acid. *Journal of Physical Chemistry A*, **2005**, 109, 2836-9	2.8	18
79	Dissociation of Difluoroethylenes. I. Global Potential Energy Surface, RRKM, and VTST Calculations. *Journal of Physical Chemistry A*, **2003**, 107, 1389-1397	2.8	18
78	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
77	l-Cysteine Modified by S-Sulfation: Consequence on Fragmentation Processes Elucidated by Tandem Mass Spectrometry and Chemical Dynamics Simulations. *Journal of Physical Chemistry A*, **2019**, 123, 3685-3696	2.8	16

76	Ab Initio Calculations on the Vinyl Fluoride Fragmentation Reactions. *Structural Chemistry*, **2001**, 12, 95-108	1.8	16
75	New interpretation of ground- and excited-state tunneling splitting in 2-pyridone/2-hydroxypyridine. *Chemical Physics Letters*, **2004**, 386, 396-402	2.5	15
74	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
73	Nonstatistical effects in the unimolecular dissociation of the acetyl radical. *Journal of Chemical Physics*, **1999**, 110, 11323-11334	3.9	15
72	GAFit: A general-purpose, user-friendly program for fitting potential energy surfaces. *Computer Physics Communications*, **2017**, 217, 89-98	4.2	14
71	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
70	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
69	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
68	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
67	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
66	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
65	Direct dynamics study of the photodissociation of triplet propanal at threshold. *Chemical Physics Letters*, **2003**, 381, 37-44	2.5	12
64	A direct DFT dynamics study of the photodissociation of triplet acetaldehyde. *Chemical Physics Letters*, **2003**, 375, 591-597	2.5	12
63	A direct classical trajectory study of the acetone photodissociation on the triplet surface. *Journal of Chemical Physics*, **2003**, 119, 10618-10625	3.9	12
62	Classical Dynamics Study of the Unimolecular Decomposition of CH3SH+. *Journal of Physical Chemistry A*, **1999**, 103, 9783-9793	2.8	11
61	DFT and Kinetic Monte Carlo Study of TMS-Substituted Ruthenium Vinyl Carbenes: Key Intermediates for Stereoselective Cyclizations. *ACS Catalysis*, **2015**, 5, 6255-6262	13.1	10
60	Femtochemistry under scrutiny: Clocking state-resolved channels in the photodissociation of CHI in the A-band. *Journal of Chemical Physics*, **2020**, 152, 014304	3.9	10
59	A comparison of X-ray and calculated structures of the enzyme MTH1. *Journal of Molecular Modeling*, **2016**, 22, 168	2	10

58	Understanding Energy Transfer in Gas–Surface Collisions from Gas-Phase Models. *Journal of Physical Chemistry C*, **2014**, 118, 2609-2621	3.8	10
57	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
56	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
55	An ab initio study of a model compound of penicillins. *Computational and Theoretical Chemistry*, **1999**, 491, 177-185		10
54	Quasi-Classical Trajectory Dynamics Study of the Cl(P) + CH4 → HCl(v,j) + CH3 Reaction. Comparison with Experiment. *Journal of Physical Chemistry A*, **2018**, 122, 2626-2633	2.8	9
53	Dynamics of Mg+ + H2O + He: capture, collisional stabilization and collision-induced dissociation. *Journal of Physical Chemistry A*, **2010**, 114, 6472-9	2.8	9
52	Chemical Dynamics Study of NO Scattering from a Perfluorinated Self-Assembled Monolayer. *Journal of Physical Chemistry C*, **2011**, 115, 23817-23830	3.8	9
51	Direct dynamics simulation of the methanethiol cation decomposition. *Chemical Physics Letters*, **2000**, 324, 88-94	2.5	9
50	Further dynamical studies of the dissociation and elimination reactions of methyl nitrite. *Journal of Chemical Physics*, **1999**, 111, 10501-10510	3.9	9
49	Enhancing Automated Reaction Discovery with Boxed Molecular Dynamics in Energy Space. *ChemSystemsChem*, **2020**, 2, e1900024	3.1	9
48	A method for predicting individual residue contributions to enzyme specificity and binding-site energies, and its application to MTH1. *Journal of Molecular Modeling*, **2016**, 22, 259	2	8
47	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
46	Energy Transfer and Thermal Accommodation in Ozone Scattering from a Perfluorinated Self-Assembled Monolayer. *Journal of Physical Chemistry C*, **2012**, 116, 25454-25464	3.8	8
45	Further studies of the methyl nitrite cis-trans isomerization. *Journal of Chemical Physics*, **1997**, 107, 5393-5405	3.9	8
44	Symmetry groups for unit cells in solids. *Journal of Computational Chemistry*, **1998**, 19, 168-180	3.5	8
43	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
42	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
41	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

40	A quantum chemical study of aniline/ammonia clusters. Thermodynamic properties and frequency analysis. *Computational and Theoretical Chemistry*, **2000**, 497, 105-113		8
39	Dynamics of the cis□trans isomerization and Cl□O dissociation of chlorine nitrite. Classical trajectory and statistical calculations. *Physical Chemistry Chemical Physics*, **2000**, 2, 5393-5399	3.6	8
38	An examination of the nature of localized molecular orbitals and their value in understanding various phenomena that occur in organic chemistry. *Journal of Molecular Modeling*, **2018**, 25, 7	2	8
37	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
36	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
35	Ab initio and RRKM study of the elimination of HF and HCl from chlorofluoroethylene. *Chemical Physics Letters*, **2007**, 435, 176-181	2.5	7
34	Rate constants and kinetic isotope effects for Cl+CH4-□lH+CH3: a comparison between LSC-IVR and statistical theories. *Chemical Physics Letters*, **2002**, 360, 59-64	2.5	7
33	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
32	AutoMeKin2021: An open-source program for automated reaction discovery. *Journal of Computational Chemistry*, **2021**, 42, 2036-2048	3.5	7
31	Standards-based curation of a decade-old digital repository dataset of molecular information. *Journal of Cheminformatics*, **2015**, 7, 43	8.6	6
30	Translational energy distributions in the photodissociation of fluorobenzene. *Chemical Physics*, **2008**, 349, 219-225	2.3	6
29	Rate constants and isotope effects for the CH3+H2-□H4+H reaction by an approximate semiclassical initial-value representation method. *Chemical Physics Letters*, **2001**, 341, 351-357	2.5	6
28	A direct dynamics study of the H2 elimination from 2,5-dihydrofuran. *Journal of Chemical Physics*, **2001**, 115, 7872-7880	3.9	6
27	Rotational effects in the unimolecular dissociation of the acetyl radical. *Chemical Physics Letters*, **2000**, 316, 471-476	2.5	6
26	Classical Trajectory Study of the Cis□Trans Isomerization and F□O Dissociation of FONO. *Journal of Physical Chemistry A*, **1998**, 102, 8708-8715	2.8	6
25	Reply to the □Comment on "Methanol dimer formation drastically enhances hydrogen abstraction from methanol by OH at low temperature"□by D. Heard, R. Shannon, J. Gomez Martin, R. Caravan, M. Blitz, J. Plane, M. Anti□olo, M. Agundez, E. Jimenez, B. Ballesteros, A. Canosa, G. El Dib, J. Albaladejo and J. Cernicharo, Phys. Chem. Chem. Phys., 2018, 20, DOI: 10.1039/C7CP04561A.	3.6	5
24	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
23	Improved United-Atom Models for Perfluorinated Self-Assembled Monolayers. *Journal of Physical Chemistry C*, **2009**, 113, 3300-3312	3.8	5

22	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
21	ChemDyME: Kinetically Steered, Automated Mechanism Generation through Combined Molecular Dynamics and Master Equation Calculations. *Journal of Chemical Theory and Computation*, **2021**, 17, 4901-4912	6.4	5
20	Specific Reaction Parameter Multigrid POTFIT (SRP-MGPF): Automatic Generation of Sum-of-Products Form Potential Energy Surfaces for Quantum Dynamical Calculations. *Frontiers in Chemistry*, **2019**, 7, 576	5	4
19	Conformational analysis of model compounds of vitamin D by theoretical calculations. *Journal of Computational Chemistry*, **1997**, 18, 1647-1655	3.5	4
18	Rate constants for the CH3O + NO -rCH3ONO reaction by classical trajectory and canonical variational transition state theory calculations. *Journal of Physical Organic Chemistry*, **2002**, 15, 123-129	2.1	4
17	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
16	A Theoretical Study of the Dynamics of the S + c-C3H Reaction. *Journal of Physical Chemistry A*, **2002**, 106, 8811-8819	2.8	4
15	Unimolecular decomposition of CH3SH+: an ab initio and RRKM study. *Computational and Theoretical Chemistry*, **2000**, 505, 109-116		4
14	The unimolecular dissociation of the propionyl radical: A classical dynamics study. *Journal of Chemical Physics*, **2001**, 114, 3546-3553	3.9	4
13	Dinmica de reacciones unimoleculares en fase gas: Desviaciones del comportamiento estadstico. *Quimica Nova*, **2002**, 25, 579-588	1.6	4
12	Representing and selecting vibrational angular momentum states for quasiclassical trajectory chemical dynamics simulations. *Journal of Physical Chemistry A*, **2007**, 111, 10292-301	2.8	3
11	Ab initio and RRKM calculations on the dissociation of the propionyl radical. *Journal of Molecular Structure*, **2000**, 556, 123-129	3.4	3
10	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
9	Application of localized molecular orbitals to the solution of semiempirical self-consistent field equations **1996**, 58, 133		3
8	Effect of the Metal Ion on the Enantioselectivity and Linkage Isomerization of Thiosemicarbazone Helicates. *Chemistry - A European Journal*, **2017**, 23, 4884-4892	4.8	2
7	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
6	Guidelines for preservation of methodological choices in the publication of computational results: B. Semiempirical electronic structure calculations(Technical report). *Pure and Applied Chemistry*, **2000**, 72, 1449-1452	2.1	2
5	A statistical study of the methyl nitrite isomerization reaction: inverse secondary isotope effects. *Chemical Physics Letters*, **1999**, 310, 209-214	2.5	2

List of Publications

4	A DFT study of a model compound of vitamin D. *Computational and Theoretical Chemistry*, **1999**, 492, 143-150	2
3	New Tools for Taming Complex Reaction Networks: The Unimolecular Decomposition of Indole Revisited. *ACS Physical Chemistry Au*,	2
2	Symmetry groups for unit cells in solids **1998**, 19, 168	1
1	Photoisomerization of Linear and Stacked Isomers of a Charged Styryl Dye: A Tandem Ion Mobility Study. *Journal of the American Society for Mass Spectrometry*, **2021**, 32, 2842-2851	3.5