

# Bruno Martínez-Haya

## List of Publications by Year in descending order

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98  
papers

2,490  
citations

172457

29  
h-index

223800

46  
g-index

100  
all docs

100  
docs citations

100  
times ranked

2015  
citing authors

#	ARTICLE	IF	CITATIONS
1	Inclusion complexes of the macrocycle nonactin with benchmark protonated amines: aniline and serine. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 8422-8431.	2.8	0
2	Tailoring the phase diagram of discotic mesogens. <i>Soft Matter</i> , 2021, 17, 8693-8704.	2.7	1
3	Proton in the ring: spectroscopy and dynamics of proton bonding in macrocycle cavities. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21532-21543.	2.8	5
4	Molecular Characterization of Nonvolatile Fractions of Algerian Petroleum with High-Resolution Mass Spectrometry. <i>Energy &amp; Fuels</i> , 2021, 35, 8699-8710.	5.1	2
5	Dynamics of coordination of $H_3O^+$ and $NH_4^+$ in crown ether cavities. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8633-8640.	2.8	8
6	Multipodal coordination and mobility of molecular cations inside the macrocycle valinomycin. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19725-19734.	2.8	3
7	Coadsorption of Counterionic Colloids at Fluid Interfaces: A Coarse-Grained Simulation Study of Gibbs Monolayers. <i>Langmuir</i> , 2020, 36, 2877-2885.	3.5	0
8	Insights into the Recognition of Phosphate Groups by Peptidic Arginine from Action Spectroscopy and Quantum Chemical Computations. <i>Journal of Physical Chemistry A</i> , 2019, , .	2.5	0
9	Insights into the Recognition of Phosphate Groups by Peptidic Arginine from Action Spectroscopy and Quantum Chemical Computations. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7528-7535.	2.6	3
10	A Cl <sup>-</sup> Hinge for Cyclen Macrocycles: Ionic Interactions and Tweezer-Like Complexes. <i>Frontiers in Chemistry</i> , 2019, 7, 143.	3.6	1
11	Guanidinium/ammonium competition and proton transfer in the interaction of the amino acid arginine with the tetracarboxylic 18-crown-6 ionophore. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4067-4073.	2.8	16
12	Intra-cavity proton bonding and anharmonicity in the anionophore cyclen. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8968-8975.	2.8	7
13	Preferential host-guest coordination of nonactin with ammonium and hydroxylammonium. <i>Journal of Chemical Physics</i> , 2018, 149, 225101.	3.0	7
14	Complexes of Crown Ether Macrocycles with Methyl Guanidinium: Insights into the Capture of Charge in Peptides. <i>ChemPhysChem</i> , 2018, 19, 2169-2175.	2.1	4
15	Isolated alkali cation complexes of the antibiotic ionophore nonactin: correlation with crystalline structures. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 14984-14991.	2.8	4
16	Benchmark Ditopic Binding of $Cl^-$ and $Cs^+$ by the Macrocycle Hexacyclen. <i>ChemPhysChem</i> , 2017, 18, 1324-1332.	2.1	8
17	On the ionophoric selectivity of nonactin and related macrotetrolide derivatives. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 1288-1297.	2.8	6
18	Isolated complexes of the amino acid arginine with polyether and polyamine macrocycles, the role of proton transfer. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 31345-31351.	2.8	25

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19	Ab initio molecular dynamics investigation of proton delocalization in crown ether complexes with H <sub>3</sub> O <sup>+</sup> and NH <sub>4</sub> <sup>+</sup> . Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 85, 83-92.	1.6	6
20	A Comparative study of the chemical structure of asphaltenes from Algerian petroleum collected at different stages of extraction and processing. Journal of Petroleum Science and Engineering, 2016, 138, 50-56.	4.2	22
21	Enhanced cation recognition by a macrocyclic ionophore at the air/water solution interface probed by mass spectrometry. Physical Chemistry Chemical Physics, 2016, 18, 3497-3503.	2.8	7
22	Binding Selectivity of Macrocyclic Ionophores in Ionic Liquids versus Aqueous Solution and Solvent-free Conditions. ChemPhysChem, 2015, 16, 3672-3680.	2.1	5
23	The Cl + O <sub>3</sub> reaction: a detailed QCT simulation of molecular beam experiments. Physical Chemistry Chemical Physics, 2015, 17, 25471-25482.	2.8	5
24	Liquid crystal phase diagram of soft repulsive rods and its mapping on the hard repulsive reference fluid. Molecular Physics, 2015, 113, 1137-1144.	1.7	20
25	Transport of spherical colloids in layered phases of binary mixtures with rod-like particles. Soft Matter, 2015, 11, 3432-3440.	2.7	9
26	Platinum Nanoparticles as Photoactive Substrates for Mass Spectrometry and Spectroscopy Sensors. Journal of Physical Chemistry C, 2014, 118, 11432-11439.	3.1	28
27	Ultraviolet laser desorption/ionization mass spectrometry of single-core and multi-core polyaromatic hydrocarbons under variable conditions of collisional cooling: insights into the generation of molecular ions, fragments and oligomers. Journal of Mass Spectrometry, 2014, 49, 1127-1138.	1.6	7
28	Chiral Recognition of Amino Acid Enantiomers by a Crown Ether: Chiroptical IR-VCD Response and Computational Study. Journal of Physical Chemistry B, 2013, 117, 9362-9370.	2.6	31
29	Comparative study of pulsed laser cleaning applied to weathered marble surfaces. Applied Surface Science, 2013, 283, 193-201.	6.1	59
30	Cations in a Molecular Funnel: Vibrational Spectroscopy of Isolated Cyclodextrin Complexes with Alkali Metals. ChemPhysChem, 2013, 14, 400-407.	2.1	15
31	Multipodal coordination of a tetracarboxylic crown ether with NH <sub>4</sub> <sup>+</sup> : A vibrational spectroscopy and computational study. Journal of Chemical Physics, 2012, 136, 114301.	3.0	8
32	High-Resolution Rotational Spectroscopy of a Cyclic Ether. Journal of Physical Chemistry Letters, 2012, 3, 482-485.	4.6	11
33	Microwave spectroscopy and quantum chemical investigation of nine low energy conformers of the 15-crown-5 ether. Physical Chemistry Chemical Physics, 2012, 14, 12912.	2.8	15
34	Tweezer-like Complexes of Crown Ethers with Divalent Metals: Probing Cation-Size-Dependent Conformations by Vibrational Spectroscopy in the Gas Phase. ChemPlusChem, 2012, 77, 118-123.	2.8	11
35	Conformational landscape of a chiral crown ether: a vibrational circular dichroism spectroscopy and computational study. Tetrahedron: Asymmetry, 2012, 23, 294-299.	1.8	11
36	Theoretical study of the dynamics of Cl + O <sub>3</sub> reaction I. Ab initio potential energy surface and quasiclassical trajectory results. Physical Chemistry Chemical Physics, 2011, 13, 8537.	2.8	9

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37	Phase behavior of hard colloidal platelets using free energy calculations. <i>Journal of Chemical Physics</i> , 2011, 134, 094501.	3.0	59
38	Platinum Nanoparticles Prepared by Laser Ablation in Aqueous Solutions: Fabrication and Application to Laser Desorption Ionization. <i>Journal of Physical Chemistry C</i> , 2011, 115, 22217-22224.	3.1	46
39	Vibrational study of isolated 18-crown-6 ether complexes with alkaline-earth metal cations. <i>International Journal of Mass Spectrometry</i> , 2011, 308, 217-224.	1.5	45
40	Crown Ether Complexes with $H_3O^+$ and $NH_4^+$ : Proton Localization and Proton Bridge Formation. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7275-7282.	2.5	55
41	Emergence of Symmetry and Chirality in Crown Ether Complexes with Alkali Metal Cations. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7048-7054.	2.5	64
42	UV-Vis-NIR Laser Desorption/Ionization of Synthetic Polymers Assisted by Gold Nanospheres, Nanorods and Nanostars. <i>Plasmonics</i> , 2010, 5, 125-133.	3.4	28
43	Nematic stability of discotic liquid crystals with orientation-dependent interactions. <i>Physical Review E</i> , 2010, 81, 020701.	2.1	9
44	Nanoparticle $TiO_2$ Films Prepared by Pulsed Laser Deposition: Laser Desorption and Cationization of Model Adsorbates. <i>Journal of Physical Chemistry C</i> , 2010, 114, 17409-17415.	3.1	24
45	One- and Two-Step Ultraviolet and Infrared Laser Desorption Ionization Mass Spectrometry of Asphaltenes. <i>Energy &amp; Fuels</i> , 2010, 24, 6067-6073.	5.1	28
46	Gas-phase complexes of cyclic and linear polyethers with alkali cations. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 13752.	2.8	31
47	Columnar phases of discotics with orientation-dependent interactions. <i>Journal of Chemical Physics</i> , 2009, 131, 074901.	3.0	20
48	Simulation study of discotic molecules in the vicinity of the isotropic-liquid crystal transition. <i>Molecular Simulation</i> , 2009, 35, 1077-1083.	2.0	14
49	Spectroscopic Investigation of the Gas-Phase Conformations of 15-Crown-5 Ether Complexes with $K^+$ . <i>Journal of Physical Chemistry A</i> , 2009, 113, 7748-7752.	2.5	29
50	Liquid crystal phase behavior of hard oblate spherocylinders. , 2009, , .		0
51	Poly(ethylene glycol) cationization with alkali metals in matrix-assisted laser desorption ionization investigated with the solvent-free method. <i>Applied Physics A: Materials Science and Processing</i> , 2008, 92, 859-863.	2.3	9
52	Matrix-assisted laser desorption mass spectrometry of gas-phase peptide-metal complexes. <i>Applied Physics A: Materials Science and Processing</i> , 2008, 93, 935-939.	2.3	6
53	Solvent-Free MALDI Investigation of the Cationization of Linear Polyethers with Alkali Metals. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8530-8535.	2.6	31
54	Contrasting Perspective on Asphaltene Molecular Weight. This Comment vs the Overview of A. A. Herod, K. D. Bartle, and R. Kandiyoti. <i>Energy &amp; Fuels</i> , 2008, 22, 1765-1773.	5.1	159

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55	Columnar phases of discotic spherocylinders. <i>Journal of Chemical Physics</i> , 2008, 129, 214706.	3.0	40
56	Use of Parsons-Lee and Onsager theories to predict nematic and demixing behavior in binary mixtures of hard rods and hard spheres. <i>Physical Review E</i> , 2007, 75, 061701.	2.1	37
57	Fragmentation and Gas Phase Aggregation Processes in the Laser Desorption/Ionization of Chlorodiaminotriazines. <i>European Journal of Mass Spectrometry</i> , 2007, 13, 321-329.	1.0	1
58	Stability of Nematic and Smectic Phases in Rod-Like Mesogens with Orientation-Dependent Attractive Interactions. <i>Journal of Physical Chemistry B</i> , 2007, 111, 8150-8157.	2.6	33
59	Molecular-Weight Distributions of Coal and Petroleum Asphaltenes from Laser Desorption/Ionization Experiments. <i>Energy &amp; Fuels</i> , 2007, 21, 2863-2868.	5.1	150
60	Laser desorption/ionization determination of molecular weight distributions of polyaromatic carbonaceous compounds and their aggregates. <i>Journal of Mass Spectrometry</i> , 2007, 42, 701-713.	1.6	78
61	Characterization and Langmuir film properties of asphaltenes extracted from Arabian light crude oil. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2007, 298, 72-79.	4.7	35
62	Matrix-Assisted laser desorption/ionization detection of carbonaceous compounds in ionic liquid matrices. <i>Rapid Communications in Mass Spectrometry</i> , 2007, 21, 3161-3164.	1.5	17
63	On the determination of molecular weight distributions of asphaltenes and their aggregates in laser desorption ionization experiments. <i>Journal of Mass Spectrometry</i> , 2006, 41, 960-968.	1.6	127
64	Freezing of hard spheres confined in narrow cylindrical pores. <i>Journal of Chemical Physics</i> , 2006, 125, 144702.	3.0	28
65	Effect of Macromolecular Crowding on the Conformation of Confined Chain Polymers. <i>Macromolecular Theory and Simulations</i> , 2005, 14, 421-427.	1.4	13
66	Quasiclassical determination of reaction probabilities as a function of the total angular momentum. <i>Journal of Chemical Physics</i> , 2005, 123, 094101.	3.0	47
67	A novel orientation-dependent potential model for prolate mesogens. <i>Journal of Chemical Physics</i> , 2005, 122, 024908.	3.0	27
68	Low-Temperature Rotational Relaxation of CO in Self-Collisions and in Collisions with Ne and He. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9402-9413.	2.5	8
69	Parsons-Lee and Monte Carlo Study of Soft Repulsive Nematogens. <i>Journal of Physical Chemistry B</i> , 2005, 109, 13729-13736.	2.6	18
70	Photodissociation and multiphoton dissociative ionization processes in CH <sub>3</sub> S <sub>2</sub> CH <sub>3</sub> at 193 nm studied using velocity-map imaging. <i>Journal of Chemical Physics</i> , 2004, 120, 11042-11052.	3.0	21
71	Crowding effects in binary mixtures of rod-like and spherical particles. <i>Journal of Molecular Recognition</i> , 2004, 17, 417-425.	2.1	30
72	Photodissociation Dynamics of Dimethyl Sulfide Following Excitation within the First Absorption Band. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7936-7948.	2.5	10

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73	Low temperature rotational relaxation of N2 in collisions with He. <i>Chemical Physics Letters</i> , 2003, 367, 500-506.	2.6	7
74	Angular momentum alignment of Cl(2P3/2) in the 308 nm photolysis of Cl2 determined using Fourier moment velocity-map imaging. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 856-864.	2.8	47
75	Liquid crystal behavior of the Kihara fluid. <i>Physical Review E</i> , 2003, 68, 011704.	2.1	25
76	Solution of the Percus-Yevick equation for square well spherocylinders. <i>Physical Review E</i> , 2003, 67, 051201.	2.1	8
77	The O(1D)+H2 reaction at 56 meV collision energy: A comparison between quantum mechanical, quasiclassical trajectory, and crossed beam results. <i>Journal of Chemical Physics</i> , 2002, 116, 10692-10703.	3.0	74
78	Monte Carlo study of liquid crystal phases of hard and soft spherocylinders. <i>Journal of Chemical Physics</i> , 2002, 117, 2934-2946.	3.0	50
79	A quasiclassical trajectory and quantum mechanical study of the O(1D)+D2 reaction dynamics. Comparison with high resolution molecular beam experiments. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 4379-4385.	2.8	19
80	Gas phase molecular relaxation at very low temperatures. A comparative study of N2 and its mixtures with He and Ne. <i>Vacuum</i> , 2002, 64, 417-423.	3.5	7
81	The stereodynamics of the O(1D)+HD reaction on the ground $1\sigma^2$ and excited $1\sigma^3$ potential energy surfaces. <i>Journal of Chemical Physics</i> , 2001, 114, 8328-8338.	3.0	23
82	Low-Temperature Rotational Relaxation of N2 in Collisions with Ne. <i>Journal of Physical Chemistry A</i> , 2001, 105, 6976-6982.	2.5	12
83	Gibbs ensemble simulation of the vapour-liquid equilibrium of square well spherocylinders. <i>Molecular Physics</i> , 2001, 99, 509-516.	1.7	14
84	The photodissociation of CH <sub>3</sub> SCH <sub>3</sub> and CD <sub>3</sub> SCD <sub>3</sub> at 220–231 nm investigated by velocity map ion imaging. <i>Journal of Chemical Physics</i> , 2001, 114, 4450.	3.0	18
85	Photodissociation of CD <sub>3</sub> SCD <sub>3</sub> on the First Absorption Band: Translational and Internal Energy Transfer to the CD <sub>3</sub> Fragment Studied by Resonant Multiphoton Ionization and Time-of-Flight Spectrometry. <i>Journal of Physical Chemistry A</i> , 2000, 104, 10150-10158.	2.5	10
86	Analytical solution to a nonseparable interaction model for a one-dimensional fluid of anisotropic molecules near a hard wall. <i>Physical Review E</i> , 1999, 59, 1957-1967.	2.1	5
87	Low-Temperature Rotational Relaxation of N2 Studied with Resonance-Enhanced Multiphoton Ionization. <i>Journal of Physical Chemistry A</i> , 1999, 103, 823-832.	2.5	26
88	Quantum mechanical and quasiclassical trajectory study of state-to-state differential cross sections for the F+D <sub>2</sub> →DF+D reaction in the center-of-mass and laboratory frames. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 3415-3427.	2.8	39
89	Quantum mechanical and quasiclassical simulations of molecular beam experiments for the F+H <sub>2</sub> →HF+H reaction on two ab initio potential energy surfaces. <i>Journal of Chemical Physics</i> , 1998, 109, 7224-7237.	3.0	81
90	The H+D <sub>2</sub> reaction in the vicinity of the conical intersection. <i>Journal of Chemical Physics</i> , 1997, 106, 7862-7864.	3.0	37

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91	Ab Initio Simulation of Molecular Beam Experiments for the $F + H_2 \rightarrow HF + H$ Reaction. <i>Journal of Physical Chemistry A</i> , 1997, 101, 6403-6414.	2.5	59
92	Experimental Absolute Cross-Sections for the Reaction $F + D_2$ at Collision Energies 90–240 meV. <i>Journal of Physical Chemistry A</i> , 1997, 101, 6415-6428.	2.5	35
93	F-D <sub>2</sub> state resolved reactive scattering at 180 and 240 meV collision energies. I. A high resolution crossed molecular beam experiment. <i>Chemical Physics</i> , 1996, 207, 227-243.	1.9	25
94	F-D <sub>2</sub> state resolved reactive scattering at 180 and 240 meV collision energies. II. Quasi-classical cross sections. A comparison with the experimental results. <i>Chemical Physics</i> , 1996, 207, 245-259.	1.9	22
95	An intense fluorine atom beam source. <i>Journal Physics D: Applied Physics</i> , 1996, 29, 1885-1893.	2.8	14
96	New Results on the Reactive Scattering of Atomic Fluorine by Molecular Deuterium at 3.2 kcal/mol Collision Energy. <i>Zeitschrift Fur Physikalische Chemie</i> , 1995, 188, 197-214.	2.8	22
97	A scattering study of the dependence of the $F + D_2(j_i = 0, 1, 2) \rightarrow DF(v_i, j_f) + D$ reaction on the initial rotational state. <i>Chemical Physics Letters</i> , 1995, 232, 197-206.	2.6	42
98	A further test of the shape and anisotropy of the $F-H_2$ interaction potential. <i>Chemical Physics</i> , 1995, 200, 405-413.	1.9	10