Iker LeÃ³n

List of Publications by Year
in descending order

83 papers	1,191 citations	430874 18 h-index	477307 29 g-index
89 all docs	89 docs citations	89 times ranked	880 citing authors

#	Article	IF	Citations
1	The design and construction of a high-resolution velocity-map imaging apparatus for photoelectron spectroscopy studies of size-selected clusters. Review of Scientific Instruments, 2014, 85, 083106.	1.3	131
2	Dispersive soft x-ray absorption fine-structure spectroscopy in graphite with an attosecond pulse. Optica, 2018, 5, 502.	9.3	47
3	High resolution photoelectron imaging of Au2â^. Journal of Chemical Physics, 2013, 138, 184304.	3.0	46
4	Exploring microsolvation of the anesthetic propofol. Physical Chemistry Chemical Physics, 2012, 14, 4398.	2.8	40
5	Communication: Vibrational spectroscopy of Au4 from high resolution photoelectron imaging. Journal of Chemical Physics, 2013, 139, 021106.	3.0	38
6	Unravelling Proteinâ€“DNA Interactions at Molecular Level: A DFT and NCI Study. Journal of Chemical Theory and Computation, 2016, 12, 523-534.	5.3	35
7	Shaping Micelles: The Interplay Between Hydrogen Bonds and Dispersive Interactions. Angewandte Chemie - International Edition, 2013, 52, 7772-7775.	13.8	31
8	Unveiling the nâ†'Ï€* interactions in dipeptides. Communications Chemistry, 2019, 2, .	4.5	30
9	Attosecond state-resolved carrier motion in quantum materials probed by soft x-ray XANES. Applied Physics Reviews, 2021, 8, .	11.3	30
10	The role of amino acid side chains in stabilizing dipeptides: the laser ablation Fourier transform microwave spectrum of Ac-Val-NH‹sub›2‹/sub›. Physical Chemistry Chemical Physics, 2017, 19, 24985-24990.	2.8	28
11	Unveiling the Neutral Forms of Glutamine. Angewandte Chemie - International Edition, 2019, 58, 16002-16007.	13.8	27
12	Probing the electronic structure and Auâ€“C chemical bonding in AuC2â^' and AuC2 using high-resolution photoelectron spectroscopy. Journal of Chemical Physics, 2014, 140, 084303.	3.0	26
13	Mimicking anaestheticâ€“receptor interaction: a combined spectroscopic and computational study of propofolâ‹¯phenol. Physical Chemistry Chemical Physics, 2012, 14, 8956.	2.8	25
14	A Spectroscopic and Computational Study of Propofol Dimers and Their Hydrated Clusters. ChemPhysChem, 2012, 13, 3819-3826.	2.1	23
15	Modeling the tyrosineâ€“sugar interactions in supersonic expansions: glucopyranoseâ€“phenol clusters. Physical Chemistry Chemical Physics, 2016, 18, 12457-12465.	2.8	23
16	Molecular recognition in the gas phase: benzocaineâ€“phenol as a model of anaestheticâ€“receptor interaction. Physical Chemistry Chemical Physics, 2009, 11, 11608.	2.8	21
17	Mass-Resolved Infrared Spectroscopy of Complexes without Chromophore by Nonresonant Femtosecond Ionization Detection. Journal of Physical Chemistry A, 2012, 116, 6798-6803.	2.5	19
18	Isomerism of the Aniline Trimer. Angewandte Chemie - International Edition, 2018, 57, 15112-15116.	13.8	19

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19	Exploring the Maze of Cycloserine Conformers in the Gas Phase Guided by Microwave Spectroscopy and Quantum Chemistry. Journal of Physical Chemistry A, 2021, 125, 2121-2129.	2.5	19
20	A combined spectroscopic and theoretical study of propofolÂ·(H2O)3. Journal of Chemical Physics, 2012, 137, 074303.	3.0	18
21	A Spectroscopic Approach to the Solvation of Anesthetics in Jets: Propofol(H2O)n, n = 4â€“6. Journal of Physical Chemistry A, 2012, 116, 8934-8941.	2.5	18
22	Probing the electronic structure and Auâ€”C chemical bonding in AuCnâ¯ and AuCnHâ¯ (n = 2, 4, and 6) using high-resolution photoelectron spectroscopy. Journal of Chemical Physics, 2016, 145, 064304.	3.0	18
23	Axialâ€“equatorial isomerism and semiexperimental equilibrium structures of fluorocyclohexane. Physical Chemistry Chemical Physics, 2017, 19, 29162-29169.	2.8	18
24	Formation of water polyhedrons in propofolâ€“water clusters. Physical Chemistry Chemical Physics, 2013, 15, 568-575.	2.8	16
25	The Structural Signs of Sweetness in Artificial Sweeteners: A Rotational Study of Sorbitol and Dulcitol. ChemPhysChem, 2018, 19, 3334-3340.	2.1	16
26	IR mass-resolved spectroscopy of complexes without chromophore: CyclohexanolÂ·(H2O)n, n = 1â€“3 and cyclohexanol dimer. Journal of Chemical Physics, 2013, 139, 174312.	3.0	15
27	Mass resolved IR spectroscopy of anilineâ€“water aggregates. Physical Chemistry Chemical Physics, 2016, 18, 27336-27341.	2.8	15
28	Laser Ablation Assists Cyclization Reactions of Hydantoic Acid: A Proof for the Near-Attack Conformation Theory?. Journal of Physical Chemistry Letters, 2019, 10, 1325-1330.	4.6	15
29	The role of the intramolecular interactions in the structural behavior of biomolecules: Insights from rotational spectroscopy. , 2021, , 93-141.		15
30	Water Encapsulation by Nanomicelles. Angewandte Chemie - International Edition, 2014, 53, 12480-12483.	13.8	14
31	Influence of the Anomeric Conformation in the Intermolecular Interactions of Glucose. Journal of Physical Chemistry Letters, 2017, 8, 1147-1151.	4.6	14
32	The Six Isomers of the Cyclohexanol Dimer: A Delicate Test for Dispersion Models. Angewandte Chemie - International Edition, 2020, 59, 14081-14085.	13.8	14
33	Looking for the Elusive Imine Tautomer of Creatinine: Different States of Aggregation Studied by Quantum Chemistry and Molecular Spectroscopy. ChemPlusChem, 2021, 86, 1374-1386.	2.8	14
34	Influence of dispersive forces on the final shape of a reverse micelle. Physical Chemistry Chemical Physics, 2015, 17, 2241-2245.	2.8	13
35	Probing the structures and bonding of auropolyynes, Auâ€”(Câ‰¡C)nâ€”Auâ¯ (n = 1â€“3), using high-resolution photoelectron imaging. Journal of Chemical Physics, 2018, 149, 144307.	3.0	13
36	Stepwise Nucleation of Aniline: Emergence of Spectroscopic Fingerprints of the Liquid Phase. Chemistry - A European Journal, 2018, 24, 10291-10295.	3.3	12

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37	Shape of Testosterone. Journal of Physical Chemistry Letters, 2021, 12, 6983-6987.	4.6	12
38	Combined Experimental and Theoretical Study of the Benzocaine/Ar van der Waals System in Supersonic Expansions. Journal of Physical Chemistry A, 2009, 113, 982-988.	2.5	11
39	Unraveling the Benzocaineâ€“Receptor Interaction at Molecular Level Using Mass-Resolved Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 13472-13480.	2.6	11
40	Resonant photoelectron spectroscopy of Au2â¯ via a Feshbach state using high-resolution photoelectron imaging. Journal of Chemical Physics, 2013, 139, 194306.	3.0	11
41	Femtosecond Excited State Dynamics of Size Selected Neutral Molecular Clusters. Journal of Physical Chemistry Letters, 2016, 7, 2797-2802.	4.6	10
42	Glycinamide, a Glycine Precursor, Caught in the Gas Phase: A Laser-ablation Jet-cooled Rotational Study. Astrophysical Journal, 2018, 861, 70.	4.5	10
43	A rotational study of the AlaAla dipeptide. Physical Chemistry Chemical Physics, 2020, 22, 13867-13871.	2.8	10
44	Unveiling Five Naked Structures of Tartaric Acid. Angewandte Chemie - International Edition, 2021, 60, 17410-17414.	13.8	10
45	Mimicking anestheticâ€“receptor interactions in jets: the propofolâ€“isopropanol cluster. Physical Chemistry Chemical Physics, 2014, 16, 16968.	2.8	9
46	Competition between stacked and hydrogen bonded structures of cytosine aggregates. Physical Chemistry Chemical Physics, 2017, 19, 8826-8834.	2.8	9
47	Intrinsic folding of the cysteine residue: competition between folded and extended forms mediated by the â€“SH group. Physical Chemistry Chemical Physics, 2020, 22, 20284-20294.	2.8	9
48	An innovative approach for the generation of species of the interstellar medium. Angewandte Chemie - International Edition, 2021, 60, 24461-24466.	13.8	9
49	Magic Numbers in the Solvation of the Propofol Dimer. ChemPhysChem, 2013, 14, 1558-1562.	2.1	8
50	Phenyl-Î²-D-glucopyranoside and Phenyl-Î²-D-galactopyranoside Dimers: Small Structural Differences but Very Different Interactions. Frontiers in Physics, 2018, 6, .	2.1	8
51	The Laboratory Millimeter and Submillimeter Rotational Spectrum of Lactaldehyde and an Astronomical Search in Sgr B2(N), Orion-KL, and NGC 6334I. Astrophysical Journal, 2019, 883, 18.	4.5	8
52	Unveiling the Neutral Forms of Glutamine. Angewandte Chemie, 2019, 131, 16148-16153.	2.0	8
53	Elucidating the multiple structures of pipecolic acid by rotational spectroscopy. Physical Chemistry Chemical Physics, 2019, 21, 4155-4161.	2.8	8
54	Shapeâ€Shifting Molecules: Unveiling the Valence Tautomerism Phenomena in Bare Barbaralones. Angewandte Chemie - International Edition, 2022, 61, .	13.8	8

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55	Sugarâ€“peptidic bond interactions: spectroscopic characterization of a model system. Physical Chemistry Chemical Physics, 2017, 19, 12013-12021.	2.8	7
56	The Shape of the Archetypical Oxocarbon Squaric Acid and Its Water Clusters. Chemistry - A European Journal, 2019, 25, 10748-10755.	3.3	7
57	Revisiting the Spectroscopy of Water Dimer in Jets. Journal of Physical Chemistry Letters, 2021, 12, 1316-1320.	4.6	7
58	Millimetre-wave laboratory study of glycinamide and a search for it with ALMA towards Sagittarius B2(N). Astronomy and Astrophysics, 2022, 657, A99.	5.1	7
59	Isomerism of the Aniline Trimer. Angewandte Chemie, 2018, 130, 15332-15336.	2.0	6
60	Understanding the role of tyrosine in glycogenin. Molecular BioSystems, 2017, 13, 1709-1712.	2.9	5
61	Excited state dynamics of aniline homoclusters. Physical Chemistry Chemical Physics, 2019, 21, 3098-3105.	2.8	5
62	Rotational Spectrum of Saccharin: Structure and Sweetness. Journal of Physical Chemistry A, 2019, 123, 2756-2761.	2.5	5
63	Rotational spectroscopic study and astronomical search for propiolamide in Sgr B2(N). Astronomy and Astrophysics, 2021, 647, A55.	5.1	5
64	Molecular hydration of propofol dimers in supersonic expansions: formation of active centre-like structures. Physical Chemistry Chemical Physics, 2014, 16, 23301-23307.	2.8	4
65	The last link of the x-aminobutyric acid series: the five conformers of Î²-aminobutyric acid. Physical Chemistry Chemical Physics, 2018, 20, 15574-15580.	2.8	4
66	Laboratory Detection of Cyanoacetic Acid: A Jet-cooled Rotational Study. Astrophysical Journal, 2021, 915, 76.	4.5	4
67	Formation of interstellar cyanoacetamide: a rotational and computational study. Astronomy and Astrophysics, 2020, 644, A3.	5.1	4
68	Transition from Planar to Nonplanar Hydrogen Bond Networks in the Solvation of Aromatic Dimers: Propofol2-(H2O)2â€“4. Journal of Physical Chemistry A, 2013, 117, 3396-3404.	2.5	3
69	Behind the Reactivity of Lactones: A Computational and Spectroscopic Study of PhenolÂ·Î³-Butyrolactone. Journal of Physical Chemistry A, 2014, 118, 2568-2575.	2.5	3
70	An innovative approach for the generation of species of the interstellar medium. Angewandte Chemie, 0, , .	2.0	3
71	The effect of N-methylation on the conformational landscape of alanine: the case of N-methyl-l-alanine. Physical Chemistry Chemical Physics, 2018, 20, 29159-29165.	2.8	2
72	Influence of the solvent in the electronic excitation of aromatic alcohols: Excited state IR-UV of propofol(H2O)8. Journal of Chemical Physics, 2019, 150, 214306.	3.0	2

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73	Unleashing the shape of l-DOPA at last. Physical Chemistry Chemical Physics, 2022, 24, 3546-3554.	2.8	2
74	Computational study on the affinity of potential drugs to SARS-CoV-2 main protease. Journal of Physics Condensed Matter, 2022, 34, 294005.	1.8	2
75	Gasâ€Phase Conformational Map of the Amino Acid Isovaline. ChemPhysChem, 2020, 21, 525-530.	2.1	1
76	Rotational Spectrum and Conformational Analysis of Perillartine: Insights into the Structureâ€“Sweetness Relationship. Molecules, 2022, 27, 1924.	3.8	1
77	Evaluation of the aggregation process in a mixture of propofol and benzocaine. Physical Chemistry Chemical Physics, 2019, 21, 3537-3544.	2.8	0
78	Frontispiece: Unveiling the Neutral Forms of Glutamine. Angewandte Chemie - International Edition, 2019, 58, .	13.8	0
79	Frontispiz: Unveiling the Neutral Forms of Glutamine. Angewandte Chemie, 2019, 131, .	2.0	0
80	Noncovalent interactions in isolated molecular aggregates: From single molecules to nanostructures. , 2021, , 143-188.		0
81	Unveiling Five Naked Structures of Tartaric Acid. Angewandte Chemie, 2021, 133, 17550-17554.	2.0	0
82	The Six Isomers of the Cyclohexanol Dimer: A Delicate Test for Dispersion Models. Angewandte Chemie, 2020, 132, 14185-14189.	2.0	0
83	Shapeâ€Shifting Molecules: Unveiling the Valence Tautomerism Phenomena in Bare Barbaralones. Angewandte Chemie, 0, , .	2.0	0