

Ignacio Funes-Ardoiz

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

49 papers	1,088 citations	19 h-index	31 g-index
56 ext. papers	1,446 ext. citations	8.7 avg, IF	5.02 L-index

#	Paper	IF	Citations
49	Redox Non-innocent Ligand Controls Water Oxidation Overpotential in a New Family of Mononuclear Cu-Based Efficient Catalysts. <i>Journal of the American Chemical Society</i> , 2015 , 137, 6758-61	16.4	210
48	GoodVibes: automated thermochemistry for heterogeneous computational chemistry data. <i>F1000Research</i> , 9 , 291	3.6	74
47	Oxidative Coupling Mechanisms: Current State of Understanding. <i>ACS Catalysis</i> , 2018 , 8, 1161-1172	13.1	56
46	Single Electron Transfer Steps in Water Oxidation Catalysis. Redefining the Mechanistic Scenario. <i>ACS Catalysis</i> , 2017 , 7, 1712-1719	13.1	51
45	Copper-Catalyzed N-F Bond Activation for Uniform Intramolecular C-H Amination Yielding Pyrrolidines and Piperidines. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 8912-8916	16.4	45
44	Elucidating the Mechanism of Aryl Aminations Mediated by NHC-Supported Nickel Complexes: Evidence for a Nonradical Ni(0)/Ni(II) Pathway. <i>ACS Catalysis</i> , 2018 , 8, 3733-3742	13.1	41
43	Orthogonal Nanoparticle Catalysis with Organogermanes. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 17788-17795	16.4	41
42	Cooperative Reductive Elimination: The Missing Piece in the Oxidative-Coupling Mechanistic Puzzle. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 2764-7	16.4	38
41	Modular and Selective Arylation of Aryl Germanes (C-GeEt ₃) over C-Bpin, C-SiR ₃ and Halogens Enabled by Light-Activated Gold Catalysis. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 15543-15548	16.4	37
40	Halide Abstraction Competes with Oxidative Addition in the Reactions of Aryl Halides with [Ni(PMe ₃ Ph) ₃]. <i>Chemistry - A European Journal</i> , 2017 , 23, 16728-16733	4.8	36
39	Rational Design and Synthesis of Efficient Sunscreens To Boost the Solar Protection Factor. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 2632-2635	16.4	35
38	Oxazolone-Based Photoswitches: Synthesis and Properties. <i>European Journal of Organic Chemistry</i> , 2013 , 2013, 6611-6618	3.2	31
37	DFT Rationalization of the Diverse Outcomes of the Iodine(III)-Mediated Oxidative Amination of Alkenes. <i>Chemistry - A European Journal</i> , 2016 , 22, 7545-53	4.8	31
36	Benzylideneoxazolones as photoswitches: photochemistry and theoretical calculations. <i>Tetrahedron</i> , 2013 , 69, 9766-9771	2.4	23
35	Computational Characterization of the Mechanism for the Oxidative Coupling of Benzoic Acid and Alkynes by Rhodium/Copper and Rhodium/Silver Systems. <i>Chemistry - A European Journal</i> , 2018 , 24, 12383-12388	4.8	28
34	Established and Emerging Computational Tools to Study Homogeneous Catalysis From Quantum Mechanics to Machine Learning. <i>CheM</i> , 2020 , 6, 1904-1913	16.2	20
33	Palladium-Catalyzed Aerobic Homocoupling of Alkynes: Full Mechanistic Characterization of a More Complex Oxidase-Type Behavior. <i>ACS Catalysis</i> , 2018 , 8, 7495-7506	13.1	20

32	Selective ortho-Functionalization of Adamantylarenes Enabled by Dispersion and an Air-Stable Palladium(I) Dimer. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 7721-7725	16.4	19
31	Functionalization of C _n H _{2n+2} Alkanes: Supercritical Carbon Dioxide Enhances the Reactivity towards Primary Carbon-Hydrogen Bonds. <i>ChemCatChem</i> , 2015 , 7, 3254-3260	5.2	19
30	Four Oxidation States in a Single Photoredox Nickel-Based Catalytic Cycle: A Computational Study. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 3898-3902	16.4	17
29	Orthogonal Nanoparticle Catalysis with Organogermanes. <i>Angewandte Chemie</i> , 2019 , 131, 17952-17959	3.6	17
28	Photocontrolled Cobalt Catalysis for Selective Hydroboration of α,β -Unsaturated Ketones. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 21176-21182	16.4	16
27	Catalytic Enantio- and Diastereoselective Mannich Addition of TosMIC to Ketimines. <i>Chemistry - A European Journal</i> , 2018 , 24, 17660-17664	4.8	15
26	Consecutive Ligand-Based Electron Transfer in New Molecular Copper-Based Water Oxidation Catalysts. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 18639-18644	16.4	14
25	Enantioselective Synthesis of Aminodiols by Sequential Rhodium-Catalysed Oxyamination/Kinetic Resolution: Expanding the Substrate Scope of Amidine-Based Catalysis. <i>Chemistry - A European Journal</i> , 2018 , 24, 4635-4642	4.8	13
24	Understanding the Mechanism of the Divergent Reactivity of Non-Heteroatom-Stabilized Chromium Carbene Complexes with Furfural Imines: Formation of Benzofurans and Azetines. <i>Journal of Organic Chemistry</i> , 2016 , 81, 1565-70	4.2	13
23	Intermolecular and regioselective access to polysubstituted benzo- and dihydrobenzo[c]azepine derivatives: modulating the reactivity of group 6 non-heteroatom-stabilized alkynyl carbene complexes. <i>Chemistry - A European Journal</i> , 2014 , 20, 7061-8	4.8	12
22	Hydroalkylation of Unactivated Olefins via Visible-Light-Driven Dual Hydrogen Atom Transfer Catalysis. <i>Journal of the American Chemical Society</i> , 2021 , 143, 11251-11261	16.4	12
21	Cooperative Reductive Elimination: The Missing Piece in the Oxidative-Coupling Mechanistic Puzzle. <i>Angewandte Chemie</i> , 2016 , 128, 2814-2817	3.6	11
20	Unexpected [4 + 2] Cycloaddition through Chromium Non-Heteroatom-Stabilized Alkynyl Carbene Complexes: Regioselective Access to Substituted 6-Azaindoles. <i>Organic Letters</i> , 2018 , 20, 4099-4102	6.2	10
19	Accelerated Ru-Cu Trinuclear Cooperative C-H Bond Functionalization of Carbazoles: A Kinetic and Computational Investigation. <i>Chemistry - A European Journal</i> , 2018 , 24, 15178-15184	4.8	9
18	Computational Characterization of Single-Electron Transfer Steps in Water Oxidation. <i>Inorganics</i> , 2019 , 7, 32	2.9	8
17	Modular and Selective Arylation of Aryl Germanes (C ₆ Et ₃) over CBpin, CBiR ₃ and Halogens Enabled by Light-Activated Gold Catalysis. <i>Angewandte Chemie</i> , 2020 , 132, 15673-15678	3.6	8
16	The Role of Electron-Donor Substituents in the Family of OPBAN-Cu Water Oxidation Catalysts: Effect on the Degradation Pathways and Efficiency. <i>European Journal of Inorganic Chemistry</i> , 2019 , 2019, 2109-2114	2.3	7
15	Selective ortho-Functionalization of Adamantylarenes Enabled by Dispersion and an Air-Stable Palladium(I) Dimer. <i>Angewandte Chemie</i> , 2020 , 132, 7795-7799	3.6	7

14	Computational assessment of non-heteroatom-stabilized carbene complexes reactivity: formation of oxazine derivatives. <i>Journal of Organic Chemistry</i> , 2014 , 79, 11824-8	4.2	7
13	Accelerated dinuclear palladium catalyst identification through unsupervised machine learning. <i>Science</i> , 2021 , 374, 1134-1140	33.3	7
12	Rational Design and Synthesis of Efficient Sunscreens To Boost the Solar Protection Factor. <i>Angewandte Chemie</i> , 2017 , 129, 2676-2679	3.6	6
11	GARLEEK: Adding an extra flavor to ONIOM. <i>Journal of Computational Chemistry</i> , 2019 , 40, 381-386	3.5	6
10	Stability of Hierarchically Formed Titanium(IV) Tris(catecholate ester) Helicates with Cyclohexyl Substituents in DMSO. <i>Inorganic Chemistry</i> , 2020 , 59, 1758-1762	5.1	5
9	On the mechanism of the Shapiro reaction: understanding the regioselectivity. <i>RSC Advances</i> , 2015 , 5, 37292-37297	3.7	4
8	Enantioselective Synthesis of 3-Heterosubstituted-2-amino-1-ols by Sequential Metal-Free Diene Aziridination/Kinetic Resolution. <i>Chemistry - A European Journal</i> , 2019 , 25, 12628-12635	4.8	3
7	Four Oxidation States in a Single Photoredox Nickel-Based Catalytic Cycle: A Computational Study. <i>Angewandte Chemie</i> , 2019 , 131, 3938-3942	3.6	2
6	Work-hardening Photopolymer from Renewable Photoactive 3,3'-(2,5-Furandiyl)bisacrylic Acid. <i>ChemSusChem</i> , 2020 , 13, 4140-4150	8.3	2
5	Dual Photoredox/Cobaloxime Catalysis for Cross-Dehydrogenative C-Heteroarylation of Amines. <i>Organic Letters</i> , 2021 , 23, 5378-5382	6.2	2
4	Consecutive Ligand-Based Electron Transfer in New Molecular Copper-Based Water Oxidation Catalysts. <i>Angewandte Chemie</i> , 2021 , 133, 18787-18792	3.6	2
3	Mechanistic Studies on the Synthesis of Pyrrolidines and Piperidines via Copper-Catalyzed Intramolecular C-H Amination.. <i>Organometallics</i> , 2022 , 41, 1099-1105	3.8	1
2	Modular access to substituted cyclohexanes with kinetic stereocontrol.. <i>Science</i> , 2022 , 376, 749-753	33.3	1
1	On the Use of Thermodynamic Cycles for the Calculation of Standard Potentials for the Oxidation of Solid Metals in Solution. <i>ChemPhysChem</i> , 2019 , 20, 159-162	3.2	