Ainara Nova

List of Publications by Year
in descending order

60 papers	3,219 citations	136950 32 h-index	149698 56 g-index
63 all docs	63 docs citations	63 times ranked	3605 citing authors

#	Article	IF	Citations
1	Iridium-Catalyzed Hydrogenation of N-Heterocyclic Compounds under Mild Conditions by an Outer-Sphere Pathway. Journal of the American Chemical Society, 2011, 133, 7547-7562.	13.7	296
2	Merging Sustainability with Organocatalysis in the Formation of Organic Carbonates by Using CO₂ as a Feedstock. ChemSusChem, 2012, 5, 2032-2038.	6.8	283
3	Mechanism of Homogeneous Iridium-Catalyzed Alkylation of Amines with Alcohols from a DFT Study. Organometallics, 2008, 27, 2529-2535.	2.3	149
4	Hydrogenation of CO₂ to Methanol by Pt Nanoparticles Encapsulated in UiO-67: Deciphering the Role of the Metalâ€“Organic Framework. Journal of the American Chemical Society, 2020, 142, 999-1009.	13.7	141
5	Design of a Versatile and Improved Precatalyst Scaffold for Palladium-Catalyzed Cross-Coupling: (Î·³-1-^tBu-indenyl)₂(Î¼-Cl)₂Pd₂. ACS Catalysis, 2015, 5, 3680-3688.	11.2	133
6	Mechanistic Study of an Improved Ni Precatalyst for Suzukiâ€“Miyaura Reactions of Aryl Sulfamates: Understanding the Role of Ni(I) Species. Journal of the American Chemical Society, 2017, 139, 922-936.	13.7	130
7	Breaking Câ€“F Bonds via Nucleophilic Attack of Coordinated Ligands: Transformations from Câ€“F to Câ€“X Bonds (X= H, N, O, S). Organometallics, 2012, 31, 1245-1256.	2.3	110
8	Enantioselective Incorporation of CO₂: Status and Potential. ACS Catalysis, 2017, 7, 7231-7244.	11.2	105
9	An Experimentalâˆ’Theoretical Study of the Factors That Affect the Switch between Ruthenium-Catalyzed Dehydrogenative Amide Formation versus Amine Alkylation. Organometallics, 2010, 29, 6548-6558.	2.3	103
10	Competing Câˆ’F Activation Pathways in the Reaction of Pt(0) with Fluoropyridines: Phosphine-Assistance versus Oxidative Addition. Journal of the American Chemical Society, 2008, 130, 15499-15511.	13.7	101
11	A Critical Analysis of the Cyclic and Open Alternatives of the Transmetalation Step in the Stille Cross-Coupling Reaction. Journal of the American Chemical Society, 2006, 128, 14571-14578.	13.7	100
12	Understanding Precatalyst Activation in Cross-Coupling Reactions: Alcohol Facilitated Reduction from Pd(II) to Pd(0) in Precatalysts of the Type (Î·3-allyl)Pd(L)(Cl) and (Î·3-indenyl)Pd(L)(Cl). ACS Catalysis, 2015, 5, 5596-5606.	11.2	89
13	Selective Activation of the <i>ortho</i> Câˆ’F Bond in Pentafluoropyridine by Zerovalent Nickel: Reaction via a Metallophosphorane Intermediate Stabilized by Neighboring Group Assistance from the Pyridyl Nitrogen. Organometallics, 2010, 29, 1824-1831.	2.3	87
14	Synthesis of PCPâ€Supported Nickel Complexes and their Reactivity with Carbon Dioxide. Chemistry - A European Journal, 2012, 18, 6915-6927.	3.3	73
15	Designing Pd and Ni Catalysts for Cross-Coupling Reactions by Minimizing Off-Cycle Species. ACS Catalysis, 2018, 8, 3499-3515.	11.2	72
16	Influence of Defects and H₂O on the Hydrogenation of CO₂ to Methanol over Pt Nanoparticles in UiO-67 Metalâ€“Organic Framework. Journal of the American Chemical Society, 2020, 142, 17105-17118.	13.7	68
17	Nickel(I) Monomers and Dimers with Cyclopentadienyl and Indenyl Ligands. Chemistry - A European Journal, 2014, 20, 5327-5337.	3.3	65
18	A Gold Exchange: A Mechanistic Study of a Reversible, Formal Ethylene Insertion into a Gold(III)â€“Oxygen Bond. Journal of the American Chemical Society, 2014, 136, 10104-10115.	13.7	64

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19	How Solvent Dynamics Controls the Schlenk Equilibrium of Grignard Reagents: A Computational Study of CH₃MgCl in Tetrahydrofuran. Journal of Physical Chemistry B, 2017, 121, 4226-4237.	2.6	63
20	Mâ•NÎ±Cycloaddition and NÎ±âˆ’NÎ²Insertion in the Reactions of Titanium Hydrazido Compounds with Alkynes: A Combined Experimental and Computational Study. Journal of the American Chemical Society, 2010, 132, 10484-10497.	13.7	53
21	The Key Role of the Hemiaminal Intermediate in the Iron-Catalyzed Deaminative Hydrogenation of Amides. ACS Catalysis, 2018, 8, 8751-8762.	11.2	53
22	Reaction Site Diversity in the Reactions of Titanium Hydrazides with Organic Nitriles, Isonitriles and Isocyanates: Tiï£¾N_{Î±} Cycloaddition, Tiï£¾N_{Î±} Insertion and N_{Î±}ï£¿N_{Î²} Bond Cleavage. Chemistry - A European Journal, 2011, 17, 265-285.	3.3	52
23	Formation of a Vinyliminium Palladium Complex by Câˆ’C Coupling in Vinylcarbene Palladium Aryl Complexes. Organometallics, 2006, 25, 1293-1297.	2.3	42
24	Observation of a Hidden Intermediate in the Stille Reaction. Study of the Reversal of the Transmetalation Step. Journal of the American Chemical Society, 2008, 130, 10518-10520.	13.7	42
25	Reactions of Cyclopentadienylâˆ’Amidinate Titanium Hydrazides with CO₂, CS₂, and Isocyanates: Tiâ•N_{Î±} Cycloaddition, Cycloadditionâˆ’Insertion, and Cycloadditionâˆ’NNR₂ Group Transfer Reactions. Organometallics, 2011, 30, 1182-1201.	2.3	41
26	Highly selective hydrogenation of amides catalysed by a molybdenum pincer complex: scope and mechanism. Chemical Science, 2019, 10, 10566-10576.	7.4	41
27	Computational Studies Explain the Importance of Two Different Substituents on the Chelating Bis(amido) Ligand for Transfer Hydrogenation by Bifunctional Cp*Rh(III) Catalysts. Organometallics, 2014, 33, 3433-3442.	2.3	39
28	Single and double substrate insertion into the Tiî€N_{Î±}bonds of terminal titanium hydrazides. Chemical Communications, 2010, 46, 85-87.	4.1	37
29	An Unusual Example of Hypervalent Silicon: A Fiveâ€Coordinate Silyl Group Bridging Two Palladium or Nickel Centers through a Nonsymmetrical Fourâ€Center Twoâ€Electron Bond. Angewandte Chemie - International Edition, 2014, 53, 1103-1108.	13.8	37
30	Synthesis and structure of â€œ16-electronâ€•rhodium(iii) catalysts for transfer hydrogenation of a cyclic imine: mechanistic implications. Chemical Communications, 2009, , 6801.	4.1	35
31	<i>trans</i>-Mutation at Gold(III): A Mechanistic Study of a Catalytic Acetylene Functionalization via a Double Insertion Pathway. ACS Catalysis, 2017, 7, 5023-5034.	11.2	35
32	Siâ€“H and Siâ€“Cl bond activation reactions of titanium hydrazides with silanes and subsequent Tiâ€“H/Eâ€“H (E = Si or H) Ïƒ-bond metathesis. Chemical Communications, 2011, 47, 3147.	4.1	32
33	Site selectivity and reversibility in the reactions of titanium hydrazides with Siâ€“H, Siâ€“X, Câ€“X and H+ reagents: Tiî€NÎ± 1,2-silane addition, NÎ² alkylation, NÎ± protonation and Ïƒ-bond metathesis. Dalton Transactions, 2012, 41, 2277.	3.3	32
34	Deciphering Selectivity in Organic Reactions: A Multifaceted Problem. Accounts of Chemical Research, 2016, 49, 1070-1078.	15.6	31
35	Csp3â€“F bond activation by nucleophilic attack of the {Pt2S2} core assisted by non-covalent interactions. Chemical Communications, 2008, , 3130.	4.1	26
36	Aromatic Câ€“F activation by complexes containing the {Pt2S2} core via nucleophilic substitution: a combined experimental and theoretical study. Dalton Transactions, 2009, , 5980.	3.3	24

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37	Behavior of Pâˆ’Pt and Pâˆ’Pd Bonds in Phosphido Complexes toward Electrophilic Fragments. Inorganic Chemistry, 2009, 48, 7679-7690.	4.0	23
38	Synthesis and Reactions of a Cyclopentadienyl-Amidinate Titanium <i>tert-</i>Butoxyimido Compound. Organometallics, 2013, 32, 7520-7539.	2.3	21
39	Mild, Reversible Reaction of Iridium(III) Amido Complexes with Carbon Dioxide. Inorganic Chemistry, 2012, 51, 9683-9693.	4.0	20
40	Coordination and insertion of alkenes and alkynes in Au^{III}complexes: nature of the intermediates from a computational perspective. Dalton Transactions, 2016, 45, 5504-5513.	3.3	20
41	Synthesis of a (N,C,C) Au(<scp>iii</scp>) pincer complex <i>via</i> C_{sp3}â€“H bond activation: increasing catalyst robustness by rational catalyst design. Chemical Communications, 2018, 54, 11104-11107.	4.1	20
42	Titanium alkoxyimido (Tiî€Nâ€“OR) complexes: reductive Nâ€“O bond cleavage at the boundary between hydrazide and peroxide ligands. Chemical Communications, 2011, 47, 4926.	4.1	19
43	A Highly Asymmetric Gold(III) Î·³â€Allyl Complex. Angewandte Chemie - International Edition, 2020, 59, 1516-1520.	13.8	18
44	Câ€“S Bond Activation and Partial Hydrogenation of Thiophene by a Dinuclear Trihydride Platinum Complex. European Journal of Inorganic Chemistry, 2007, 2007, 5707-5719.	2.0	17
45	Mechanism of the Rhodiumâ€Catalyzed Asymmetric Isomerization of Allylamines to Enamines. Chemistry - A European Journal, 2008, 14, 3323-3329.	3.3	17
46	Does the metal protect the ancillary ligands? Câ€“H strengthening and deactivation in amines and phosphines upon metal-binding. Chemical Communications, 2014, 50, 614-616.	4.1	17
47	Cu-catalyzed <i>N</i>-3-Arylation of Hydantoins Using Diaryliodonium Salts. Organic Letters, 2020, 22, 2687-2691.	4.6	16
48	Titanium <i>tert</i>-Butoxyimido Compounds. Inorganic Chemistry, 2011, 50, 12155-12171.	4.0	15
49	Small-molecule activation at Au(iii): metallacycle construction from ethylene, water, and acetonitrile. Dalton Transactions, 2016, 45, 14719-14724.	3.3	15
50	DFT Investigation of Suzukiâ€“Miyaura Reactions with Aryl Sulfamates Using a Dialkylbiarylphosphine-Ligated Palladium Catalyst. Organometallics, 2017, 36, 3664-3675.	2.3	15
51	Rational selection of co-catalysts for the deaminative hydrogenation of amides. Chemical Science, 2020, 11, 2225-2230.	7.4	13
52	Aliphatic Câ€“X (X=halogen) bond activation by transition metal complexes containing the {Pt2S2} core: A theoretical study of the reaction mechanism. Inorganica Chimica Acta, 2006, 359, 3736-3744.	2.4	12
53	The mechanism of N-vinylindole formation via tandem imine formation and cycloisomerisation of o-ethynylanilines. Dalton Transactions, 2009, , 10296.	3.3	10
54	A Combined Experimental/Computational Study of the Mechanism of a Palladiumâ€Catalyzed Boraâ€Negishi Reaction. Chemistry - A European Journal, 2017, 23, 12655-12667.	3.3	8

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55	Unmasking the constitution and bonding of the proposed lithium nickelate â€œLi₃NiPh₃(solv)₃â€ revealing the hidden C₆H₄ligand. Chemical Science, 2022, 13, 5268-5276.	7.4	8
56	Synthesis and Characterization of Stable Gold(III) PNP Pincer Complexes. European Journal of Inorganic Chemistry, 2018, 2018, 3113-3117.	2.0	7
57	Synthesis, Characterization, and Reactivity of Cyclometalated Gold(III) Dihalide Complexes in <i>Aqua Regia</i>. European Journal of Inorganic Chemistry, 2020, 2020, 3249-3258.	2.0	5
58	Synthesis of substituted (N,C) and (N,C,C) Au(<scp>iii</scp>) complexes: the influence of sterics and electronics on cyclometalation reactions. Dalton Transactions, 2022, 51, 5082-5097.	3.3	5
59	Computational Studies on the Mechanisms for Deaminative Amide Hydrogenation by Homogeneous Bifunctional Catalysts. Topics in Catalysis, 2022, 65, 82-95.	2.8	5
60	A Highly Asymmetric Gold(III) Î· 3 â€Allyl Complex. Angewandte Chemie, 2020, 132, 1532-1536.	2.0	4