

# Agusti Lledos

## List of Publications by Year in Descending Order

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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.

372  
papers

11,788  
citations

54  
h-index

79  
g-index

404  
ext. papers

12,539  
ext. citations

6.9  
avg, IF

6.29  
L-index

#	Paper	IF	Citations
372	Copper(I) activation of C-X bonds: bimolecular unimolecular reaction mechanism.. <i>Chemical Communications</i> , <b>2022</b> ,	5.8	1
371	Understanding the Use of Phosphine-(EWO) Ligands in Negishi Cross-Coupling: Experimental and Density Functional Theory Mechanistic Study. <i>Organometallics</i> , <b>2021</b> , 40, 2272-2282	3.8	2
370	Computational Organometallic Catalysis: Where We Are, Where We Are Going. <i>European Journal of Inorganic Chemistry</i> , <b>2021</b> , 2021, 2547-2555	2.3	9
369	Transmetalation Reactions Triggered by Electron Transfer between Organocopper Complexes. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 11633-11639	5.1	3
368	Computational Analysis on the Pd-Catalyzed C-N Coupling of Ammonia with Aryl Bromides Using a Chelate Phosphine Ligand. <i>Journal of Organic Chemistry</i> , <b>2021</b> , 86, 4007-4017	4.2	4
367	Ligand Effects in Carbon-Boron Coupling Processes Mediated by EBH Platinum Complexes. <i>European Journal of Inorganic Chemistry</i> , <b>2021</b> , 2021, 3528-3539	2.3	0
366	Design and evolution of chimeric streptavidin for protein-enabled dual gold catalysis. <i>Nature Catalysis</i> , <b>2021</b> , 4, 643-653	36.5	4
365	How acid can become a dihydrogen complex in water? A DFT study. <i>Journal of Organometallic Chemistry</i> , <b>2021</b> , 949, 121957	2.3	0
364	Dynamic Pd /Cu Multimetallic Assemblies as Molecular Models to Study Metal-Metal Cooperation in Sonogashira Coupling. <i>Chemistry - A European Journal</i> , <b>2020</b> , 26, 12168-12179	4.8	10
363	Molecular Modeling for Artificial Metalloenzyme Design and Optimization. <i>Accounts of Chemical Research</i> , <b>2020</b> , 53, 896-905	24.3	17
362	Catalytic Regioselective Isomerization of 2,2-Disubstituted Oxetanes to Homoallylic Alcohols. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 7591-7597	3.6	
361	Catalytic Regioselective Isomerization of 2,2-Disubstituted Oxetanes to Homoallylic Alcohols. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 7521-7527	16.4	7
360	Skeletal diversity in Pt- and Au-catalyzed annulations of allenedienes: dissecting unconventional mechanistic pathways. <i>Chemical Science</i> , <b>2020</b> , 11, 4209-4220	9.4	1
359	What Makes a Good (Computed) Energy Profile?. <i>Topics in Organometallic Chemistry</i> , <b>2020</b> , 1-38	0.6	9
358	Aerobic intramolecular carbon-hydrogen bond oxidation promoted by Cu(I) complexes. <i>Dalton Transactions</i> , <b>2020</b> , 49, 14647-14655	4.3	4
357	Comparative Mechanistic Study on the [Au(NHC)] <sup>+</sup> -Catalyzed Hydration of Alkynes, Alkenes, and Allenes. <i>Organometallics</i> , <b>2020</b> , 39, 3469-3479	3.8	6
356	Reversible carbon-boron bond formation at platinum centers through EBH complexes. <i>Chemical Science</i> , <b>2020</b> , 12, 1647-1655	9.4	3

355	Ambiphilic boryl groups in a neutral Ni(II) complex: a new activation mode of H <sub>2</sub> . <i>Chemical Science</i> , <b>2020</b> , 12, 2540-2548	9.4	3
354	Et <sub>3</sub> Si <sub>2</sub> Platinum(II) Complexes as Intermediates in C-Si Bond-Coupling Processes. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 11346-11355	4.8	6
353	Mild Iridium-Catalysed Isomerization of Epoxides. Computational Insights and Application to the Synthesis of $\beta$ -Alkyl Amines. <i>Advanced Synthesis and Catalysis</i> , <b>2019</b> , 361, 3624-3631	5.6	4
352	The Effect of Cofactor Binding on the Conformational Plasticity of the Biological Receptors in Artificial Metalloenzymes: The Case Study of LmrR. <i>Frontiers in Chemistry</i> , <b>2019</b> , 7, 211	5	8
351	Integrated Computational Study of the Cu-Catalyzed Hydration of Alkenes in Water Solvent and into the Context of an Artificial Metallohydratase. <i>ACS Catalysis</i> , <b>2019</b> , 9, 4616-4626	13.1	7
350	Inner-Sphere Oxygen Activation Promoting Outer-Sphere Nucleophilic Attack on Olefins. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 14546-14554	4.8	5
349	Bonding rearrangements in organometallic reactions: from orbitals to curly arrows. <i>Dalton Transactions</i> , <b>2019</b> , 48, 15740-15752	4.3	10
348	Activating a Peroxo Ligand for C-O Bond Formation. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 3037-3041	16.4	5
347	Origin of the Anti-Markovnikov Hydroamination of Alkenes Catalyzed by LAu(I) Complexes: Coordination Mode Determines Regioselectivity. <i>ACS Catalysis</i> , <b>2019</b> , 9, 848-858	13.1	26
346	Activating a Peroxo Ligand for C=O Bond Formation. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 3069-3073	3.6	2
345	GARLEEK: Adding an extra flavor to ONIOM. <i>Journal of Computational Chemistry</i> , <b>2019</b> , 40, 381-386	3.5	6
344	Decoding Surface Interaction of VO Metallo-drug Candidates with Lysozyme. <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 4456-4469	5.1	22
343	Computational Studies of Artificial Metalloenzymes: From Methods and Models to Design and Optimization <b>2018</b> , 99-136		2
342	Well-Defined $\beta$ -Diketiminatocobalt(II) Complexes for Alkene Cyclohydroamination of Primary Amines. <i>ACS Catalysis</i> , <b>2018</b> , 8, 4446-4451	13.1	11
341	Isolation of a Cationic Platinum(II) Et <sub>3</sub> Si <sub>2</sub> Complex. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 3271-3275	3.6	7
340	Isolation of a Cationic Platinum(II) Et <sub>3</sub> Si <sub>2</sub> Complex. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 3217-3221	16.4	19
339	Calculation of Reaction Free Energies in Solution: A Comparison of Current Approaches. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 1392-1399	2.8	82
338	An Artificial Heme Enzyme for Cyclopropanation Reactions. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 7911-7915	3.6	19

- 337 An Artificial Heme Enzyme for Cyclopropanation Reactions. *Angewandte Chemie - International Edition*, **2018**, 57, 7785-7789 16.4 72
- 336 Prediction of the interaction of metallic moieties with proteins: An update for protein-ligand docking techniques. *Journal of Computational Chemistry*, **2018**, 39, 42-51 3.5 44
- 335 Selective Synthesis of Tetrasubstituted Olefins by Copper-Mediated Acetoxythiolation of Internal Alkynes: Scope and Mechanistic Studies. *Chemistry - A European Journal*, **2018**, 24, 13124-13135 4.8 10
- 334 Direct Asymmetric Hydrogenation of N-Methyl and N-Alkyl Imines with an Ir(III)H Catalyst. *Journal of the American Chemical Society*, **2018**, 140, 16967-16970 16.4 36
- 333 Iridium-Catalyzed Isomerization of N-Sulfonyl Aziridines to Allyl Amines. *Organic Letters*, **2018**, 20, 5747-5751 18
- 332 Accurate prediction of vertical electronic transitions of Ni(II) coordination compounds via time dependent density functional theory. *International Journal of Quantum Chemistry*, **2018**, 118, e25655 2.1 7
- 331 Mechanistic Insights on the Hydration of Terminal and Internal Allenes Catalyzed by [(NHC)Au]<sup>+</sup>. *Organometallics*, **2018**, 37, 3543-3551 3.8 9
- 330 Desulfinylation of Ag(I) Sulfinyl Mesoionic Carbenes: Preparation of C-Unsubstituted Au(I)-1,2,3-Triazole Carbene Complexes. *Organic Letters*, **2017**, 19, 822-825 6.2 14
- 329 Rhodium Complexes Promoting C-O Bond Formation in Reactions with Oxygen: The Role of Superoxo Species. *Chemistry - A European Journal*, **2017**, 23, 5232-5243 4.8 6
- 328 Speciation of ZnMe<sub>2</sub>, ZnMeCl, and ZnCl<sub>2</sub> in Tetrahydrofuran (THF), and Its Influence on Mechanism Calculations of Catalytic Processes. *ACS Catalysis*, **2017**, 7, 3575-3583 13.1 24
- 327 Elucidation of Binding Site and Chiral Specificity of Oxidovanadium Drugs with Lysozyme through Theoretical Calculations. *Inorganic Chemistry*, **2017**, 56, 12938-12951 5.1 33
- 326 A competing, dual mechanism for catalytic direct benzene hydroxylation from combined experimental-DFT studies. *Chemical Science*, **2017**, 8, 8373-8383 9.4 19
- 325 Design of an enantioselective artificial metallo-hydratase enzyme containing an unnatural metal-binding amino acid. *Chemical Science*, **2017**, 8, 7228-7235 9.4 55
- 324 Computing the arrows of chemical reactions. *ChemTexts*, **2017**, 3, 1 2.2 8
- 323 Mechanistic implications of the enantioselective addition of alkylzinc reagents to aldehydes catalyzed by nickel complexes with amino amide ligands. *Organic and Biomolecular Chemistry*, **2016**, 14, 11125-11136 3.9 5
- 322 NH-Heterocyclic Aryliodonium Salts and their Selective Conversion into N1-Aryl-5-iodoimidazoles. *Angewandte Chemie - International Edition*, **2016**, 55, 7152-6 16.4 32
- 321 First-Principles Molecular Dynamics Studies of Organometallic Complexes and Homogeneous Catalytic Processes. *Accounts of Chemical Research*, **2016**, 49, 1271-8 24.3 52
- 320 The Origin of Anti-Markovnikov Regioselectivity in Alkene Hydroamination Reactions Catalyzed by [Rh(DPEphos)](L). *Chemistry - A European Journal*, **2016**, 22, 9311-20 4.8 24

319	Silver(I)-Catalyzed Addition of Phenols to Alkyne Cobalt Cluster Stabilized Carbocations. <i>Chemistry - A European Journal</i> , <b>2016</b> , 22, 9015-23	4.8	6
318	Acid Activation in Phenyliodine Dicarboxylates: Direct Observation, Structures, and Implications. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 12747-12750	16.4	93
317	Platinum(0)-mediated C-O bond activation of ethers via an S <sub>2</sub> mechanism. <i>Dalton Transactions</i> , <b>2016</b> , 45, 18842-18850	4.3	4
316	New Insights into the Reactivity of Cisplatin with Free and Restrained Nucleophiles: Microsolvation Effects and Base Selectivity in Cisplatin-DNA Interactions. <i>ChemPhysChem</i> , <b>2016</b> , 17, 3932-3947	3.2	10
315	Ketone Hydrogenation with Iridium Complexes with $\sigma$ -Bond NHC Ligands: The Key Role of the Strong Base. <i>ACS Catalysis</i> , <b>2015</b> , 5, 4368-4376	13.1	26
314	Ruthenium-Catalyzed Oxidative Coupling of Primary Amines with Internal Alkynes through C-H Bond Activation: Scope and Mechanistic Studies. <i>Chemistry - A European Journal</i> , <b>2015</b> , 21, 8626-36	4.8	33
313	Azole Assisted C-H Bond Activation Promoted by an Osmium-Polyhydride: Discerning between N and NH. <i>Organometallics</i> , <b>2015</b> , 34, 1898-1910	3.8	26
312	Toward the Computational Design of Artificial Metalloenzymes: From Protein-Ligand Docking to Multiscale Approaches. <i>ACS Catalysis</i> , <b>2015</b> , 5, 2469-2480	13.1	42
311	Realistic Simulation of Organometallic Reactivity in Solution by Means of First-Principles Molecular Dynamics. <i>Structure and Bonding</i> , <b>2015</b> , 81-106	0.9	7
310	Mechanistic Insight into the Facilitation of $\beta$ -Lactam Fragmentation through Metal Assistance. <i>Chemistry - A European Journal</i> , <b>2015</b> , 21, 16781-5	4.8	22
309	Hydroamination of C=C Multiple Bonds with Hydrazine Catalyzed by N-Heterocyclic Carbene-Gold(I) Complexes: Substrate and Ligand Effects. <i>ACS Catalysis</i> , <b>2015</b> , 5, 815-829	13.1	43
308	Palladium monophosphine Pd(PPh <sub>3</sub> ): is it really accessible in solution?. <i>Chemical Communications</i> , <b>2014</b> , 50, 661-3	5.8	28
307	Selective Catalytic Deuterium Labeling of Alcohols during a Transfer Hydrogenation Process of Ketones Using D <sub>2</sub> O as the Only Deuterium Source. Theoretical and Experimental Demonstration of a Ru <sup>II</sup> /D <sup>+</sup> Exchange as the Key Step. <i>ACS Catalysis</i> , <b>2014</b> , 4, 1040-1053	13.1	41
306	Reactivity of coordinatively unsaturated bis(N-heterocyclic carbene) Pt(II) complexes toward H <sub>2</sub> . Crystal structure of a 14-electron Pt(II) hydride complex. <i>Inorganic Chemistry</i> , <b>2014</b> , 53, 4257-68	5.1	23
305	Unravelling novel synergies between organometallic and biological partners: a quantum mechanics/molecular mechanics study of an artificial metalloenzyme. <i>Journal of the Royal Society Interface</i> , <b>2014</b> , 11,	4.1	10
304	Challenges in modelling homogeneous catalysis: new answers from ab initio molecular dynamics to the controversy over the Wacker process. <i>Chemical Society Reviews</i> , <b>2014</b> , 43, 4940-52	58.5	50
303	Structural, kinetic, and docking studies of artificial imine reductases based on biotin-streptavidin technology: an induced lock-and-key hypothesis. <i>Journal of the American Chemical Society</i> , <b>2014</b> , 136, 15676-83	16.4	59
302	A stable, mononuclear, cationic Pt(III) complex stabilised by bulky N-heterocyclic carbenes. <i>Chemical Communications</i> , <b>2014</b> , 50, 1299-301	5.8	18

301	Synthesis, structure, and catalytic applications for ortho- and meta-carboranyl based NBN pincer-Pd complexes. <i>Inorganic Chemistry</i> , <b>2014</b> , 53, 9284-95	5.1	46
300	On the road to MM'X polymers: redox properties of heterometallic Ni/Pt paddlewheel complexes. <i>Inorganic Chemistry</i> , <b>2014</b> , 53, 10553-62	5.1	4
299	Counteranion-Dependent Reaction Pathways in the Protonation of Cationic Ruthenium(Vinylidene) Complexes. <i>Organometallics</i> , <b>2014</b> , 33, 2549-2560	3.8	6
298	Computational Insights on an Artificial Imine Reductase Based on the Biotin-Streptavidin Technology. <i>ACS Catalysis</i> , <b>2014</b> , 4, 833-842	13.1	24
297	The use of localised orbitals for the bonding and mechanistic analysis of organometallic compounds. <i>Dalton Transactions</i> , <b>2014</b> , 43, 11145-51	4.3	38
296	Assessing protein-ligand docking for the binding of organometallic compounds to proteins. <i>Journal of Computational Chemistry</i> , <b>2014</b> , 35, 192-8	3.5	17
295	The Transmetalation Process in Suzuki-Miyaura Reactions: Calculations Indicate Lower Barrier via Boronate Intermediate. <i>ChemCatChem</i> , <b>2014</b> , 6, 3132-3138	5.2	55
294	Coordinatively Unsaturated T-Shaped Platinum(II) Complexes Stabilized by Small N-Heterocyclic Carbene Ligands. Synthesis and Cyclometalation. <i>Organometallics</i> , <b>2014</b> , 33, 3746-3756	3.8	20
293	Orbital-Like Motion of Hydride Ligands around Low-Coordinate Metal Centers. <i>Angewandte Chemie</i> , <b>2014</b> , 126, 14382-14385	3.6	2
292	Orbital-like motion of hydride ligands around low-coordinate metal centers. <i>Angewandte Chemie - International Edition</i> , <b>2014</b> , 53, 14158-61	16.4	12
291	Computational perspective on Pd-catalyzed C-C cross-coupling reaction mechanisms. <i>Accounts of Chemical Research</i> , <b>2013</b> , 46, 2626-34	24.3	253
290	Mechanistic studies on the Pd-catalyzed vinylation of aryl halides with vinylalkoxysilanes in water: the effect of the solvent and NaOH promoter. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 13749-63	16.4	42
289	Speciation of [Cp*(2)M(2)O(5)] in polar and donor solvents. <i>Chemistry - A European Journal</i> , <b>2013</b> , 19, 3969-85	4.8	1
288	Counteranion and solvent assistance in ruthenium-mediated alkyne to vinylidene isomerizations. <i>Inorganic Chemistry</i> , <b>2013</b> , 52, 8919-32	5.1	34
287	Solution dynamics of agostic interactions in T-shaped Pt(II) complexes from ab initio molecular dynamics simulations. <i>Dalton Transactions</i> , <b>2013</b> , 42, 12165-72	4.3	22
286	Introducing copper as catalyst for oxidative alkane dehydrogenation. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 3887-96	16.4	66
285	Mechanistic intricacies of gold-catalyzed intermolecular cycloadditions between allenamides and dienes. <i>Chemistry - A European Journal</i> , <b>2013</b> , 19, 15248-60	4.8	55
284	True and masked three-coordinate T-shaped platinum(II) intermediates. <i>Beilstein Journal of Organic Chemistry</i> , <b>2013</b> , 9, 1352-82	2.5	49

283	Incorporation of manganese complexes into xylanase: new artificial metalloenzymes for enantioselective epoxidation. <i>ChemBioChem</i> , <b>2012</b> , 13, 240-51	3.8	65
282	A versatile Ru catalyst for the asymmetric transfer hydrogenation of both aromatic and aliphatic sulfinylimines. <i>Chemistry - A European Journal</i> , <b>2012</b> , 18, 1969-83	4.8	49
281	Mechanistic Exploration of the Pd-Catalyzed Copper-Free Sonogashira Reaction. <i>ACS Catalysis</i> , <b>2012</b> , 2, 135-144	13.1	90
280	Pt(II) as a proton shuttle during C-H bond activation in the Shilov process. <i>Chemical Communications</i> , <b>2012</b> , 48, 1979-81	5.8	24
279	Rearrangement of Tridentate [OSO]-Type Ligands and Migratory Insertion Reaction Mechanisms in Cyclopentadienyl Tantalum Complexes. <i>Organometallics</i> , <b>2012</b> , 31, 7052-7062	3.8	5
278	Cobalt-catalyzed vinylation of aromatic halides using $\eta^5$ -halostyrene: experimental and DFT studies. <i>Journal of Organic Chemistry</i> , <b>2012</b> , 77, 5056-62	4.2	41
277	Experimental and Theoretical Studies of the Hydrogenation of $\mu$ -Unsaturated Acids by an 18e Hydride Carbonylniobocene Complex. <i>Organometallics</i> , <b>2012</b> , 31, 5177-5184	3.8	7
276	Coordination Chemistry of New Chiral P,N Ferrocenyl Ligands with Half-Sandwich Ruthenium(II), Rhodium(III), and Iridium(III) Complexes. <i>Organometallics</i> , <b>2012</b> , 31, 6669-6680	3.8	24
275	Characterization of a paramagnetic, mononuclear Pt(III)-alkyl complex intermediate in carbon-halogen bond coupling reactions. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 15261-4	16.4	27
274	Imidazole Based Ruthenium(IV) Complexes as Highly Efficient Bifunctional Catalysts for the Redox Isomerization of Allylic Alcohols in Aqueous Medium: Water as Cooperating Ligand. <i>ACS Catalysis</i> , <b>2012</b> , 2, 2087-2099	13.1	52
273	Breaking C $\sigma$ Bonds via Nucleophilic Attack of Coordinated Ligands: Transformations from C $\sigma$ to C $\pi$ Bonds (X= H, N, O, S). <i>Organometallics</i> , <b>2012</b> , 31, 1245-1256	3.8	96
272	Hydrogen/deuterium exchange in hydride chemistry: Dihydrogen bonded complexes as key intermediates. <i>Computational and Theoretical Chemistry</i> , <b>2012</b> , 998, 129-140	2	16
271	Computational insights on the possibility of tri-coordinated cisplatinated adducts with protein models. <i>Journal of Inorganic Biochemistry</i> , <b>2012</b> , 117, 230-6	4.2	4
270	Tuning N-Heterocyclic Carbenes in T-Shaped Pt(II) Complexes for Intermolecular C-H Bond Activation of Arenes. <i>Angewandte Chemie</i> , <b>2012</b> , 124, 4002-4005	3.6	16
269	Tuning N-heterocyclic carbenes in T-shaped Pt(II) complexes for intermolecular C-H bond activation of arenes. <i>Angewandte Chemie - International Edition</i> , <b>2012</b> , 51, 3936-9	16.4	44
268	The nature of [PdCl(2)(C(2)H(4))(H(2)O)] as an active species in the Wacker process: new insights from ab initio molecular dynamics simulations. <i>Chemistry - A European Journal</i> , <b>2012</b> , 18, 5612-9	4.8	30
267	Highly efficient redox isomerisation of allylic alcohols catalysed by pyrazole-based ruthenium(IV) complexes in water: mechanisms of bifunctional catalysis in water. <i>Chemistry - A European Journal</i> , <b>2012</b> , 18, 7749-65	4.8	65
266	Directionality of dihydrogen bonds: the role of transition metal atoms. <i>ChemPhysChem</i> , <b>2012</b> , 13, 2677-83	7.2	21

265	Gold-catalyzed cycloadditions involving allenes: mechanistic insights from theoretical studies. <i>Topics in Current Chemistry</i> , <b>2011</b> , 302, 225-48		30
264	What can molecular modelling bring to the design of artificial inorganic cofactors?. <i>Faraday Discussions</i> , <b>2011</b> , 148, 137-59; discussion 207-28	3.6	25
263	Cationic intermediates in the Pd-catalyzed Negishi coupling. Kinetic and density functional theory study of alternative transmetalation pathways in the Me-Me coupling of ZnMe <sub>2</sub> and trans-[PdMeCl(PMePh <sub>2</sub> ) <sub>2</sub> ]. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 13519-26	16.4	60
262	Theoretical Evaluation of Phosphine Effects in Cross-Coupling Reactions. <i>Catalysis By Metal Complexes</i> , <b>2011</b> , 57-84		10
261	The importance of conformational search: a test case on the catalytic cycle of the Suzuki-Miyaura cross-coupling. <i>Theoretical Chemistry Accounts</i> , <b>2011</b> , 128, 639-646	1.9	57
260	Gold versus Silver-Catalyzed Intermolecular Hydroaminations of Alkenes and Dienes. <i>Advanced Synthesis and Catalysis</i> , <b>2011</b> , 353, 3451-3466	5.6	38
259	Do metal-water hydrogen bonds hold in solution? Insight from ab initio molecular dynamics simulations. <i>ChemPhysChem</i> , <b>2011</b> , 12, 1666-8	3.2	21
258	Acid-Base Interaction between Transition-Metal Hydrides: Dihydrogen Bonding and Dihydrogen Evolution. <i>Angewandte Chemie</i> , <b>2011</b> , 123, 1403-1406	3.6	6
257	Hydroamination of Alkynes with Ammonia: Unforeseen Role of the Gold(I) Catalyst. <i>Angewandte Chemie</i> , <b>2011</b> , 123, 11343-11347	3.6	23
256	Acid-base interaction between transition-metal hydrides: dihydrogen bonding and dihydrogen evolution. <i>Angewandte Chemie - International Edition</i> , <b>2011</b> , 50, 1367-70	16.4	42
255	Hydroamination of alkynes with ammonia: unforeseen role of the gold(I) catalyst. <i>Angewandte Chemie - International Edition</i> , <b>2011</b> , 50, 11147-51	16.4	64
254	Basic ancillary ligands promote O-O bond formation in iridium-catalyzed water oxidation: a DFT study. <i>Dalton Transactions</i> , <b>2011</b> , 40, 11241-7	4.3	40
253	Theoretical study on intramolecular allene-diene cycloadditions catalyzed by PtCl <sub>2</sub> and Au(I) complexes. <i>Dalton Transactions</i> , <b>2011</b> , 40, 11095-105	4.3	18
252	Nature of bonding in terminal borylene, alkyne, and gallylene complexes of vanadium and niobium [( $\eta^5$ -C <sub>5</sub> H <sub>5</sub> )(CO) <sub>3</sub> M(ENR <sub>2</sub> )] (M = V, Nb; E = B, Al, Ga; R = CH <sub>3</sub> , SiH <sub>3</sub> , CMe <sub>3</sub> , SiMe <sub>3</sub> ): a DFT study. <i>Inorganic Chemistry</i> , <b>2011</b> , 50, 1402-10	5.1	25
251	Internal Alkyne Isomerization to Vinylidene versus Stable $\eta^3$ -Alkyne: Theoretical and Experimental Study on the Divergence of Analogous Cp* <i>Ru</i> and Tp <i>Ru</i> Systems. <i>Organometallics</i> , <b>2011</b> , 30, 4014-4031	3.8	34
250	Inner- and Outer-Sphere Hydrogenation Mechanisms: A Computational Perspective. <i>Advances in Inorganic Chemistry</i> , <b>2010</b> , 62, 231-260	2.1	27
249	Mechanistic Comparison of Acid- and Gold(I)-Catalyzed Nucleophilic Addition Reactions to Olefins. <i>Organometallics</i> , <b>2010</b> , 29, 5919-5926	3.8	45
248	Intramolecular sigma-bond metathesis/protonolysis on zirconium(IV) and hafnium(IV) pyridylamido olefin polymerization catalyst precursors: exploring unexpected reactivity paths. <i>Inorganic Chemistry</i> , <b>2010</b> , 49, 6811-3	5.1	19



247	Proton-transfer reactions to half-sandwich ruthenium trihydride complexes bearing hemilabile P,N ligands: experimental and density functional theory studies. <i>Inorganic Chemistry</i> , <b>2010</b> , 49, 6035-57	5.1	26
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130	Why $[CpW(CO)_3]^+$ reduces $H_2$ to dihydride. <i>Chemical Communications</i> , <b>2003</b> , 850-1	5.8	7
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128	Hexakis(silyl)palladium(VI) or Palladium(II) with $\eta^2$ -Disilane Ligands? This work was supported by the Direcció General de Enseñanza Superior (DGES), grant PB98-1166-CO2-01, and the Comissionat per a Universitats i Recerca (Generalitat de Catalunya), grant SGR99-0046. Computing resources at the Centre de Supercomputació "El Cerdà" (CESCA) and Centre de Recerca Matemàtica, Barcelona.	16.4	31
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42	Intramolecular atom exchange between molecular hydrogen and hydride ligands in $\text{cis-}[\text{Fe}(\text{PR}_3)_4\text{H}(\text{H}_2)]^+$ complexes. An ab initio theoretical study. <i>Journal of the American Chemical Society</i> , <b>1992</b> , 114, 2922-2928	16.4	39
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