

Iker Del Rosal

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.

92
papers

1,763
citations

24
h-index

37
g-index

103
ext. papers

2,118
ext. citations

7.7
avg, IF

4.65
L-index

#	Paper	IF	Citations
92	Acid Activation in Phenylidone Dicarboxylates: Direct Observation, Structures, and Implications. <i>Journal of the American Chemical Society</i> , 2016 , 138, 12747-12750	16.4	93
91	Rare-earth metal alkyl and hydride complexes stabilized by a cyclen-derived [NNNN] macrocyclic ancillary ligand. <i>Journal of the American Chemical Society</i> , 2008 , 130, 6920-1	16.4	90
90	Enantiospecific C-H Activation Using Ruthenium Nanocatalysts. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 10474-7	16.4	85
89	¹⁷ O NMR gives unprecedented insights into the structure of supported catalysts and their interaction with the silica carrier. <i>Journal of the American Chemical Society</i> , 2012 , 134, 9263-75	16.4	79
88	Mechanistic Aspects of the Polymerization of Lactide Using a Highly Efficient Aluminum(III) Catalytic System. <i>Journal of the American Chemical Society</i> , 2017 , 139, 6217-6225	16.4	65
87	Heteronuclear NMR spectroscopy as a surface-selective technique: a unique look at the hydroxyl groups of alumina. <i>Chemistry - A European Journal</i> , 2014 , 20, 4038-46	4.8	61
86	Metallacyclic yttrium alkyl and hydrido complexes: synthesis, structures and catalytic activity in intermolecular olefin hydrophosphination and hydroamination. <i>Dalton Transactions</i> , 2015 , 44, 12137-48	4.3	53
85	Near-IR Two Photon Microscopy Imaging of Silica Nanoparticles Functionalized with Isolated Sensitized Yb(III) Centers. <i>Chemistry of Materials</i> , 2014 , 26, 1062-1073	9.6	53
84	Accessing Realistic Models for the WO ₃ BiO ₂ Industrial Catalyst through the Design of Organometallic Precursors. <i>ACS Catalysis</i> , 2016 , 6, 1-18	13.1	45
83	Hydrido-ruthenium cluster complexes as models for reactive surface hydrogen species of ruthenium nanoparticles. Solid-state ² H NMR and quantum chemical calculations. <i>Journal of the American Chemical Society</i> , 2010 , 132, 11759-67	16.4	41
82	Zwitterionic amidinates as effective ligands for platinum nanoparticle hydrogenation catalysts. <i>Chemical Science</i> , 2017 , 8, 2931-2941	9.4	37
81	On the track to silica-supported tungsten oxo metathesis catalysts: input from ¹⁷ O solid-state NMR. <i>Inorganic Chemistry</i> , 2013 , 52, 10119-30	5.1	37
80	Side Arm Twist on Zn-Catalyzed Hydrosilylative Reduction of CO ₂ to Formate and Methanol Equivalents with High Selectivity and Activity. <i>ACS Catalysis</i> , 2018 , 8, 4710-4718	13.1	35
79	New perspectives in organolanthanide chemistry from redox to bond metathesis: insights from theory. <i>Chemical Society Reviews</i> , 2016 , 45, 2516-43	58.5	35
78	Well-Defined Supported Mononuclear Tungsten Oxo Species as Olefin Metathesis Pre-Catalysts. <i>ACS Catalysis</i> , 2014 , 4, 4232-4241	13.1	35
77	Theoretical characterization of the surface composition of ruthenium nanoparticles in equilibrium with syngas. <i>Nanoscale</i> , 2016 , 8, 10974-92	7.7	34
76	Polymerization of rac-Lactide Using Achiral Iron Complexes: Access to Thermally Stable Stereocomplexes. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 12585-12589	16.4	33

75	From molecular complexes to complex metallic nanostructures--2H solid-state NMR studies of ruthenium-containing hydrogenation catalysts. <i>ChemPhysChem</i> , 2013 , 14, 3026-33	3.2	32
74	DFT calculations of 1H and 13C NMR chemical shifts in transition metal hydrides. <i>Dalton Transactions</i> , 2008 , 3959-70	4.3	31
73	Where does hydrogen adsorb on Ru nanoparticles? A powerful joint (2)H MAS-NMR/DFT approach. <i>ChemPhysChem</i> , 2009 , 10, 2939-42	3.2	28
72	A Density Functional Theory Study of Spectroscopic and Thermodynamic Properties of Surficial Hydrides on Ru (0001) Model Surface: The Influence of the Coordination Modes and the Coverage. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 2169-2178	3.8	27
71	Grafting of lanthanide complexes on silica surfaces: a theoretical investigation. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 6322-30	2.8	25
70	Silica-Supported Tungsten Neosilyl Oxo Precatalysts: Impact of the Podality on Activity and Stability in Olefin Metathesis. <i>Organometallics</i> , 2016 , 35, 2188-2196	3.8	24
69	Nickel Complexes with Bis(8-quinolyl)silyl Ligands. An Unusual Ni3Si2 Cluster Containing Six-Coordinate Silicon. <i>Organometallics</i> , 2010 , 29, 5544-5550	3.8	24
68	Gold(I)-Catalysed Asymmetric Hydroamination of Alkenes: A Silver- and Solvent-Dependent Enantiodivergent Reaction. <i>Chemistry - A European Journal</i> , 2017 , 23, 10777-10788	4.8	23
67	The Nature of Secondary Interactions at Electrophilic Metal Sites of Molecular and Silica-Supported Organolutetium Complexes from Solid-State NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 2016 , 138, 3831-43	16.4	23
66	Small changes have consequences: lessons from tetrabenzyltitanium and -zirconium surface organometallic chemistry. <i>Chemistry - A European Journal</i> , 2013 , 19, 964-73	4.8	23
65	DFT 2H quadrupolar coupling constants of ruthenium complexes: a good probe of the coordination of hydrides in conjunction with experiments. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 5657-63	3.6	23
64	Ligand-field theory-based analysis of the adsorption properties of ruthenium nanoparticles. <i>ACS Nano</i> , 2013 , 7, 9823-35	16.7	22
63	DFT study of the ring opening polymerization of ϵ -caprolactone by grafted lanthanide complexes: 1--Effect of the grafting mode on the reactivity of borohydride complexes. <i>Dalton Transactions</i> , 2011 , 40, 11211-27	4.3	21
62	DFT study of the ring opening polymerization of ϵ -caprolactone by grafted lanthanide complexes: 2--Effect of the initiator ligand. <i>Dalton Transactions</i> , 2011 , 40, 11228-40	4.3	21
61	DFT investigations on the ring-opening polymerization of substituted cyclic carbonates catalyzed by zinc-(μ -diketiminato) complexes. <i>Polymer Chemistry</i> , 2015 , 6, 3336-3352	4.9	20
60	Ring-opening polymerization of racemic ϵ -butyrolactone promoted by rare earth trisborohydride complexes towards a PHB-diol: an experimental and DFT study. <i>Polymer Chemistry</i> , 2013 , 4, 3077	4.9	20
59	NH formation from N and H mediated by molecular tri-iron complexes. <i>Nature Chemistry</i> , 2020 , 12, 740-746	4.6	19
58	DFT investigations on the ring-opening polymerization of cyclic carbonates catalyzed by zinc-(μ -diiminato) complexes. <i>Polymer Chemistry</i> , 2011 , 2, 2564	4.9	19

57	Ligand effect on the NMR, vibrational and structural properties of tetra- and hexanuclear ruthenium hydrido clusters: a theoretical investigation. <i>Dalton Transactions</i> , 2009 , 2142-56	4.3	18
56	Efficient CO ₂ transformation under ambient condition by heterobimetallic rare earth complexes: Experimental and computational evidences of a synergistic effect. <i>Journal of CO₂ Utilization</i> , 2019 , 33, 413-418	7.6	17
55	Functionalization of Carbon Monoxide and tert-Butyl Nitrile by Intramolecular Proton Transfer in a Bis(Phosphido) Thorium Complex. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 16748-16753	16.4	16
54	Scandium alkyl and hydride complexes supported by a pentadentate diborate ligand: reactions with CO and NO. <i>Dalton Transactions</i> , 2018 , 47, 13680-13688	4.3	16
53	Supported neodymium catalysts for MMA polymerization: on the origin of surface-induced stereoselectivity. <i>Polymer Chemistry</i> , 2012 , 3, 1730-1739	4.9	15
52	Hydrogen Isotope Exchange Catalyzed by Ru Nanocatalysts: Labelling of Complex Molecules Containing N-Heterocycles and Reaction Mechanism Insights. <i>Chemistry - A European Journal</i> , 2020 , 26, 4988-4996	4.8	15
51	Yttrium Dihydride Cation [YH ₂ (THF) ₂] ⁺ⁿ : Aggregate Formation and Reaction with (NNNN)-Type Macrocycles. <i>Organometallics</i> , 2015 , 34, 3739-3747	3.8	14
50	Comparative Insertion Reactivity of CO, CO ₂ , tBuCN, and tBuNC into Thorium and Uranium Phosphorus Bonds. <i>Organometallics</i> , 2020 , 39, 2152-2161	3.8	14
49	Shape, electronic structure and steric effects of organometallic nanocatalysts: relevant tools to improve the synergy between theory and experiment. <i>Dalton Transactions</i> , 2017 , 46, 378-395	4.3	14
48	On the Interaction of Phosphines with High Surface Area Mesoporous Silica. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 25919-25927	3.8	14
47	Carboxylic acid-capped ruthenium nanoparticles: experimental and theoretical case study with ethanoic acid. <i>Nanoscale</i> , 2019 , 11, 9392-9409	7.7	13
46	Grafting of lanthanide complexes on silica surfaces dehydroxylated at 200 °C: a theoretical investigation. <i>New Journal of Chemistry</i> , 2015 , 39, 7703-7715	3.6	13
45	To bend or not to bend: experimental and computational studies of structural preference in Ln(Tp(iPr) ₂) ₂ (Ln = Sm, Tm). <i>Inorganic Chemistry</i> , 2014 , 53, 12066-75	5.1	13
44	² H NMR calculations on polynuclear transition metal complexes: on the influence of local symmetry and other factors. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 20199-207	3.6	13
43	Single-site cobalt and zinc catalysts for the ring-opening polymerization of lactide. <i>European Polymer Journal</i> , 2019 , 120, 109208	5.2	12
42	Surprising Differences of Alkane C-H Activation Catalyzed by Ruthenium Nanoparticles: Complex Surface-Substrate Recognition?. <i>ChemCatChem</i> , 2018 , 10, 4243-4247	5.2	12
41	Amido Analogues of Nonbent Lanthanide (II) and Calcium Metallocenes. Heterolytic Cleavage of C-Bond Ln-Carbazoyl Ligand Promoted by Lewis Base Coordination. <i>Organometallics</i> , 2015 , 34, 555-562	3.8	12
40	Monomeric thorium dihydrido complexes: versatile precursors to actinide metallacycles. <i>Chemical Communications</i> , 2019 , 55, 8560-8563	5.8	11

39	Divergent uranium- phosphorus-based reduction of MeSiN with steric modification of phosphido ligands. <i>Chemical Science</i> , 2020 , 11, 5830-5835	9.4	10
38	Modification of silica-supported tungsten neosilyl oxo precatalysts: impact of substituted phenol on activity and stability in olefin metathesis. <i>Catalysis Science and Technology</i> , 2016 , 6, 8532-8539	5.5	10
37	Control of the single atom/nanoparticle ratio in Pd/C catalysts to optimize the cooperative hydrogenation of alkenes. <i>Catalysis Science and Technology</i> , 2021 , 11, 984-999	5.5	10
36	Reversing Conventional Reactivity of Mixed Oxo/Alkyl Rare-Earth Complexes: Non-Redox Oxygen Atom Transfer. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 1062-1067	16.4	10
35	Formation of an σ -Diimine from Isocyanide Coupling Using Thorium(IV) and Uranium(IV) PhosphidoMethyl Complexes. <i>Organometallics</i> , 2019 , 38, 1733-1740	3.8	9
34	Unprecedented Reaction Mode of Phosphorus in Phosphinidene Rare-Earth Complexes: A Joint Experimental-Theoretical Study. <i>Journal of the American Chemical Society</i> , 2018 , 140, 102-105	16.4	9
33	Silica-Grafted Lanthanum Benzyl Species: Synthesis, Characterization, and Catalytic Applications. <i>Organometallics</i> , 2017 , 36, 3912-3920	3.8	8
32	PMLABe diol synthesized by ring-opening polymerization of racemic benzyl β -malolactonate initiated by rare-earth trisborohydride complexes: an experimental and DFT study. <i>Chemistry - A European Journal</i> , 2014 , 20, 14387-402	4.8	8
31	Strongly Polarized Iridium-Aluminum Pairs: Unconventional Reactivity Patterns Including CO Cooperative Reductive Cleavage. <i>Journal of the American Chemical Society</i> , 2021 , 143, 4844-4856	16.4	7
30	Catalysis to discriminate single atoms from subnanometric ruthenium particles in ultra-high loading catalysts. <i>Catalysis Science and Technology</i> , 2020 , 10, 4673-4683	5.5	6
29	Molecular Thorium Trihydrido Clusters Stabilized by Cyclopentadienyl Ligands. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 11250-11255	16.4	6
28	3D Ruthenium Nanoparticle Covalent Assemblies from Polymantane Ligands for Confined Catalysis. <i>Chemistry of Materials</i> , 2020 , 32, 2365-2378	9.6	6
27	Mechanistic Studies on the Catalytic Synthesis of BN Heterocycles (1H-2,1-Benzazaboroles) at Ruthenium. <i>ACS Catalysis</i> , 2018 , 8, 939-948	13.1	6
26	O MAS NMR studies of oxo-based olefin metathesis catalysts: a critical assessment of signal enhancement methods. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 28157-28163	3.6	6
25	Effects of the Grafting of Lanthanum Complexes on a Silica Surface on the Reactivity: Influence on Ethylene, Propylene, and 1,3-Butadiene Homopolymerization. <i>Inorganic Chemistry</i> , 2016 , 55, 10024-10033	5.1	5
24	Nickel(0)-Induced β -H Elimination of Magnesium Alkyls: Formation and Reactivity of Heterometallic Hydrides. <i>Inorganic Chemistry</i> , 2020 , 59, 13473-13480	5.1	5
23	Uncatalyzed Formation of Polyaminoboranes from Diisopropylaminoborane and Primary Amines: a Kinetically Controlled Polymerization Reaction. <i>Advanced Synthesis and Catalysis</i> , 2021 , 363, 2417-2426	5.6	5
22	Rationalizing the Reactivity of Mixed Allyl Rare-Earth Borohydride Complexes with DFT Studies. <i>Catalysts</i> , 2020 , 10, 820	4	4

21	Stepwise construction of silica-supported tantalum/iridium heteropolymetallic catalysts using surface organometallic chemistry. <i>Journal of Catalysis</i> , 2020 , 392, 287-301	7.3	4
20	Alternative (E)-arene vs. (E,N,N) coordination of a sterically demanding amidinate ligand: are size and electronic structure of the Ln ion decisive factors?. <i>Dalton Transactions</i> , 2019 , 48, 8317-8326	4.3	3
19	DFT calculations in periodic boundary conditions of gas-phase acidities and of transition-metal anionic clusters: case study with carboxylate-stabilized ruthenium clusters. <i>Theoretical Chemistry Accounts</i> , 2019 , 138, 1	1.9	3
18	A Uranium(II) Arene Complex That Acts as a Uranium(I) Synthone. <i>Journal of the American Chemical Society</i> , 2021 , 143, 19748-19760	16.4	3
17	A combined theoretical/experimental study highlighting the formation of carbides on Ru nanoparticles during CO hydrogenation. <i>Nanoscale</i> , 2021 , 13, 6902-6915	7.7	3
16	Grafting of a new bis-silylamido aluminum species on silica: insight from solid-state NMR into interactions with the surface. <i>Dalton Transactions</i> , 2019 , 48, 5243-5252	4.3	2
15	Multicentered effective group potentials: ligand-field effects in organometallic clusters and dynamical study of chemical reactivity. <i>Theoretical Chemistry Accounts</i> , 2010 , 126, 151-163	1.9	2
14	Two-Electron Reduction of a U(VI) Complex with Al(CMe). <i>Inorganic Chemistry</i> , 2020 , 59, 16137-16142	5.1	2
13	Calcium-mediated C(sp)-H Activation and Alkylation of Alkylpyridines. <i>Inorganic Chemistry</i> , 2021 , 60, 5114-5121	4.5	2
12	Sabatier Principle and Surface Properties of Small Ruthenium Nanoparticles and Clusters: Case Studies 2021 , 331-351		2
11	Mechanistic investigations via DFT support the cooperative heterobimetallic C-H and O-H bond activation across Ta[double bond, length as m-dash]Ir multiple bonds. <i>Dalton Transactions</i> , 2021 , 50, 504-510	4.3	2
10	Hydrosilylative reduction of carbon dioxide by a homoleptic lanthanum aryloxide catalyst with high activity and selectivity. <i>Dalton Transactions</i> , 2021 , 50, 7804-7809	4.3	2
9	How CuI and NaI Interact with Faujasite Zeolite? A Theoretical Investigation. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 28026-28037	3.8	1
8	Grafting of Lanthanum Complexes on a Functionalized Graphene Surface: Theoretical Investigation on Ethylene and 1,3-Butadiene Homo- and Co-Polymerization. <i>Chemistry - A European Journal</i> , 2020 , 26, 13213-13225	4.8	1
7	When organophosphorus ruthenium complexes covalently bind to ruthenium nanoparticles to form nanoscale hybrid materials. <i>Chemical Communications</i> , 2020 , 56, 4059-4062	5.8	1
6	Molecular Thorium Trihydrido Clusters Stabilized by Cyclopentadienyl Ligands. <i>Angewandte Chemie</i> , 2020 , 132, 11346-11351	3.6	1
5	Speciation of [Cp*(2)M(2)O(5)] in polar and donor solvents. <i>Chemistry - A European Journal</i> , 2013 , 19, 3969-85	4.8	1
4	Synthesis, Characterization, and Comparative Theoretical Investigation of Dinitrogen-Bridged Group 6-Gold Heterobimetallic Complexes. <i>Inorganic Chemistry</i> , 2021 , 60, 5545-5562	5.1	1

3	Bimetallic RuNi nanoparticles as catalysts for upgrading biomass: metal dilution and solvent effects on selectivity shifts. <i>Green Chemistry</i> ,	10	1
2	Scandium and lanthanum hydride complexes stabilized by super-bulky penta-arylcyclopentadienyl ligands. <i>Chemical Communications</i> , 2021 , 57, 7766-7769	5.8	1
1	Surface reactions of ammonia on ruthenium nanoparticles revealed by ¹⁵ N and ¹³ C solid-state NMR. <i>Catalysis Science and Technology</i> , 2021 , 11, 4509-4520	5.5	0