

Iker Del Rosal

List of Publications by Year in descending order

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99
papers

2,427
citations

186209

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103
all docs

103
docs citations

103
times ranked

2401
citing authors

#	ARTICLE	IF	CITATIONS
1	Acid Activation in Phenyliodine Dicarboxylates: Direct Observation, Structures, and Implications. <i>Journal of the American Chemical Society</i> , 2016, 138, 12747-12750.	6.6	127
2	Enantiospecific C-H Activation Using Ruthenium Nanocatalysts. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 10474-10477.	7.2	118
3	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, 6920-6921.	6.6	99
4	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, 9263-9275.	6.6	93
5	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.	6.6	85
6	Heteronuclear NMR Spectroscopy as a Surface-Selective Technique: A Unique Look at the Hydroxyl Groups of γ -Alumina. <i>Chemistry - A European Journal</i> , 2014, 20, 4038-4046.	1.7	82
7	Metallacyclic yttrium alkyl and hydrido complexes: synthesis, structures and catalytic activity in intermolecular olefin hydrophosphination and hydroamination. <i>Dalton Transactions</i> , 2015, 44, 12137-12148.	1.6	65
8	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.	3.2	61
9	Accessing Realistic Models for the WO ₃ -SiO ₂ Industrial Catalyst through the Design of Organometallic Precursors. <i>ACS Catalysis</i> , 2016, 6, 1-18.	5.5	54
10	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.	5.5	51
11	Zwitterionic amidinates as effective ligands for platinum nanoparticle hydrogenation catalysts. <i>Chemical Science</i> , 2017, 8, 2931-2941.	3.7	48
12	Polymerization of rac-Lactide Using Achiral Iron Complexes: Access to Thermally Stable Stereocomplexes. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 12585-12589.	7.2	47
13	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, 11759-11767.	6.6	44
14	New perspectives in organolanthanide chemistry from redox to bond metathesis: insights from theory. <i>Chemical Society Reviews</i> , 2016, 45, 2516-2543.	18.7	44
15	Theoretical characterization of the surface composition of ruthenium nanoparticles in equilibrium with syngas. <i>Nanoscale</i> , 2016, 8, 10974-10992.	2.8	43
16	NH ₃ formation from N ₂ and H ₂ mediated by molecular tri-iron complexes. <i>Nature Chemistry</i> , 2020, 12, 740-746.	6.6	42
17	On the Track to Silica-Supported Tungsten Oxo Metathesis Catalysts: Input from ¹⁷ O Solid-State NMR. <i>Inorganic Chemistry</i> , 2013, 52, 10119-10130.	1.9	40
18	Well-Defined Supported Mononuclear Tungsten Oxo Species as Olefin Metathesis Pre-Catalysts. <i>ACS Catalysis</i> , 2014, 4, 4232-4241.	5.5	38

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19	DFT calculations of ¹ H and ¹³ C NMR chemical shifts in transition metal hydrides. Dalton Transactions, 2008, , 3959.	1.6	37
20	From Molecular Complexes to Complex Metallic Nanostructuresâ€” ² H Solidâ€‘State NMR Studies of Rutheniumâ€‘Containing Hydrogenation Catalysts. ChemPhysChem, 2013, 14, 3026-3033.	1.0	37
21	The Nature of Secondary Interactions at Electrophilic Metal Sites of Molecular and Silica-Supported Organolutetium Complexes from Solid-State NMR Spectroscopy. Journal of the American Chemical Society, 2016, 138, 3831-3843.	6.6	35
22	A Uranium(II) Arene Complex That Acts as a Uranium(I) Synthon. Journal of the American Chemical Society, 2021, 143, 19748-19760.	6.6	34
23	Silica-Supported Tungsten Neosilyl Oxo Precatalysts: Impact of the Podality on Activity and Stability in Olefin Metathesis. Organometallics, 2016, 35, 2188-2196.	1.1	31
24	Gold(I)â€‘Catalysed Asymmetric Hydroamination of Alkenes: Aâ€‘...Silverâ€‘and Solventâ€‘Dependent Enantiodivergent Reaction. Chemistry - A European Journal, 2017, 23, 10777-10788.	1.7	31
25	Strongly Polarized Iridium ⁺ â€‘Aluminum ⁺ Pairs: Unconventional Reactivity Patterns Including CO ₂ Cooperative Reductive Cleavage. Journal of the American Chemical Society, 2021, 143, 4844-4856.	6.6	31
26	Where does Hydrogen Adsorb on Ru Nanoparticles? A Powerful Joint ² H MASâ€‘NMR/DFT Approach. ChemPhysChem, 2009, 10, 2939-2942.	1.0	30
27	A Density Functional Theory Study of Spectroscopic and Thermodynamic Properties of Surface Hydrides on Ru (0001) Model Surface: The Influence of the Coordination Modes and the Coverage. Journal of Physical Chemistry C, 2011, 115, 2169-2178.	1.5	30
28	Efficient CO ₂ transformation under ambient condition by heterobimetallic rare earth complexes: Experimental and computational evidences of a synergistic effect. Journal of CO ₂ Utilization, 2019, 33, 413-418.	3.3	30
29	Control of the single atom/nanoparticle ratio in Pd/C catalysts to optimize the cooperative hydrogenation of alkenes. Catalysis Science and Technology, 2021, 11, 984-999.	2.1	30
30	Grafting of Lanthanide Complexes on Silica Surfaces: A Theoretical Investigation. Journal of Physical Chemistry A, 2010, 114, 6322-6330.	1.1	29
31	Nickel Complexes with Bis(8-quinolyl)silyl Ligands. An Unusual Ni ₃ Si ₂ Cluster Containing Six-Coordinate Silicon. Organometallics, 2010, 29, 5544-5550.	1.1	25
32	Functionalization of Carbon Monoxide and <i>tert</i> -Butyl Nitrile by Intramolecular Proton Transfer in a Bis(Phosphido) Thorium Complex. Angewandte Chemie - International Edition, 2018, 57, 16748-16753.	7.2	25
33	DFT ² H quadrupolar coupling constants of ruthenium complexes: a good probe of the coordination of hydrides in conjunction with experiments. Physical Chemistry Chemical Physics, 2009, 11, 5657.	1.3	24
34	DFT study of the Ring Opening Polymerization of μ -caprolactone by grafted lanthanide complexes: ¹ â€‘Effect of the grafting mode on the reactivity of borohydride complexes. Dalton Transactions, 2011, 40, 11211.	1.6	24
35	Small Changes Have Consequences: Lessons from Tetrabenzyltitanium and â€‘Zirconium Surface Organometallic Chemistry. Chemistry - A European Journal, 2013, 19, 964-973.	1.7	24
36	DFT study of the Ring Opening Polymerization of μ -caprolactone by grafted lanthanide complexes: ² â€‘Effect of the initiator ligand. Dalton Transactions, 2011, 40, 11228.	1.6	23

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37	DFT investigations on the ring-opening polymerization of substituted cyclic carbonates catalyzed by zinc- $\{\hat{\eta}^2\text{-diketiminato}\}$ complexes. <i>Polymer Chemistry</i> , 2015, 6, 3336-3352.	1.9	23
38	Scandium alkyl and hydride complexes supported by a pentadentate diborate ligand: reactions with CO_2 and N_2O . <i>Dalton Transactions</i> , 2018, 47, 13680-13688.	1.6	23
39	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.	1.7	23
40	Ligand-Field Theory-Based Analysis of the Adsorption Properties of Ruthenium Nanoparticles. <i>ACS Nano</i> , 2013, 7, 9823-9835.	7.3	22
41	DFT investigations on the ring-opening polymerization of cyclic carbonates catalyzed by zinc- $\{\hat{\eta}^2\text{-diiminato}\}$ complexes. <i>Polymer Chemistry</i> , 2011, 2, 2564.	1.9	21
42	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.	1.6	20
43	Ring-opening polymerization of racemic $\hat{\eta}^2$ -butyrolactone promoted by rare earth trisborohydride complexes towards a PHB-diol: an experimental and DFT study. <i>Polymer Chemistry</i> , 2013, 4, 3077.	1.9	20
44	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.	7.2	20
45	Carboxylic acid-capped ruthenium nanoparticles: experimental and theoretical case study with ethanoic acid. <i>Nanoscale</i> , 2019, 11, 9392-9409.	2.8	19
46	Comparative Insertion Reactivity of CO , CO_2 , tBuCN , and tBuNC into Thorium and Uranium Phosphorus Bonds. <i>Organometallics</i> , 2020, 39, 2152-2161.	1.1	19
47	Supported neodymium catalysts for MMA polymerization: on the origin of surface-induced stereoselectivity. <i>Polymer Chemistry</i> , 2012, 3, 1730-1739.	1.9	18
48	Catalysis to discriminate single atoms from subnanometric ruthenium particles in ultra-high loading catalysts. <i>Catalysis Science and Technology</i> , 2020, 10, 4673-4683.	2.1	18
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.	1.6	17
50	Monomeric thorium dihydrido complexes: versatile precursors to actinide metallacycles. <i>Chemical Communications</i> , 2019, 55, 8560-8563.	2.2	17
51	Divergent uranium- versus phosphorus-based reduction of Me_3SiN_3 with steric modification of phosphido ligands. <i>Chemical Science</i> , 2020, 11, 5830-5835.	3.7	17
52	To Bend or Not To Bend: Experimental and Computational Studies of Structural Preference in $\text{Ln}(\text{Tp}^{\text{iPr}})_2$ ($\text{Ln} = \text{Sm}, \text{Tm}$). <i>Inorganic Chemistry</i> , 2014, 53, 12066-12075.	1.9	16
53	Amido Analogues of Nonbent Lanthanide (II) and Calcium Metallocenes. Heterolytic Cleavage of $\text{C}-\text{N}$ Bond in Carbazolyl Ligand Promoted by Lewis Base Coordination. <i>Organometallics</i> , 2015, 34, 555-562.	1.1	16
54	Yttrium Dihydride Cation $[\text{YH}_2(\text{THF})_2]^+$ Aggregate Formation and Reaction with (NNNN)-Type Macrocycles. <i>Organometallics</i> , 2015, 34, 3739-3747.	1.1	16

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55	Unprecedented Reaction Mode of Phosphorus in Phosphinidene Rare-Earth Complexes: A Joint Experimentalâ€”Theoretical Study. <i>Journal of the American Chemical Society</i> , 2018, 140, 102-105.	6.6	16
56	Single-site cobalt and zinc catalysts for the ring-opening polymerization of lactide. <i>European Polymer Journal</i> , 2019, 120, 109208.	2.6	16
57	2H 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.	1.3	15
58	On the Interaction of Phosphines with High Surface Area Mesoporous Silica. <i>Journal of Physical Chemistry C</i> , 2012, 116, 25919-25927.	1.5	15
59	Grafting of lanthanide complexes on silica surfaces dehydroxylated at 200 Å°C: a theoretical investigation. <i>New Journal of Chemistry</i> , 2015, 39, 7703-7715.	1.4	15
60	Surprising Differences of Alkane Câ€”H Activation Catalyzed by Ruthenium Nanoparticles: Complex Surfaceâ€”Substrate Recognition?. <i>ChemCatChem</i> , 2018, 10, 4243-4247.	1.8	15
61	Mechanistic investigations <i>via</i> DFT support the cooperative heterobimetallic Câ€”H and Oâ€”H bond activation across Taâ€” multiple bonds. <i>Dalton Transactions</i> , 2021, 50, 504-510.	1.6	13
62	Calcium-mediated C(sp ³)â€”H Activation and Alkylation of Alkylpyridines. <i>Inorganic Chemistry</i> , 2021, 60, 5114-5121.	1.9	13
63	Two-Electron Reduction of a U(VI) Complex with Al(C ₅ Me ₅). <i>Inorganic Chemistry</i> , 2020, 59, 16137-16142.	1.9	12
64	Nickel(0)-Induced Î²-H Elimination of Magnesium Alkyls: Formation and Reactivity of Heterometallic Hydrides. <i>Inorganic Chemistry</i> , 2020, 59, 13473-13480.	1.9	12
65	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.	2.1	11
66	Formation of an Î±-Diimine from Isocyanide Coupling Using Thorium(IV) and Uranium(IV) Phosphidoâ€”Methyl Complexes. <i>Organometallics</i> , 2019, 38, 1733-1740.	1.1	11
67	Stepwise construction of silica-supported tantalum/iridium heteropolymetallic catalysts using surface organometallic chemistry. <i>Journal of Catalysis</i> , 2020, 392, 287-301.	3.1	11
68	3D Ruthenium Nanoparticle Covalent Assemblies from Polymantane Ligands for Confined Catalysis. <i>Chemistry of Materials</i> , 2020, 32, 2365-2378.	3.2	11
69	Synthesis, Characterization, and Comparative Theoretical Investigation of Dinitrogen-Bridged Group 6-Gold Heterobimetallic Complexes. <i>Inorganic Chemistry</i> , 2021, 60, 5545-5562.	1.9	11
70	¹⁷ 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.	1.3	10
71	Silica-Grafted Lanthanum Benzyl Species: Synthesis, Characterization, and Catalytic Applications. <i>Organometallics</i> , 2017, 36, 3912-3920.	1.1	10
72	Molecular Thorium Trihydrido Clusters Stabilized by Cyclopentadienyl Ligands. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 11250-11255.	7.2	9

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73	A combined theoretical/experimental study highlighting the formation of carbides on Ru nanoparticles during CO hydrogenation. <i>Nanoscale</i> , 2021, 13, 6902-6915.	2.8	9
74	Hydrosilylative reduction of carbon dioxide by a homoleptic lanthanum aryloxide catalyst with high activity and selectivity. <i>Dalton Transactions</i> , 2021, 50, 7804-7809.	1.6	9
75	Bimetallic RuNi nanoparticles as catalysts for upgrading biomass: metal dilution and solvent effects on selectivity shifts. <i>Green Chemistry</i> , 2021, 23, 8480-8500.	4.6	9
76	Scandium and lanthanum hydride complexes stabilized by super-bulky penta-arylcyclopentadienyl ligands. <i>Chemical Communications</i> , 2021, 57, 7766-7769.	2.2	9
77	Computational Design of Pd Nanoclusters and Pd Single-Atom Catalysts Supported on O-Functionalized Graphene. <i>ACS Applied Nano Materials</i> , 2021, 4, 12235-12249.	2.4	9
78	Rational Preparation of Well-Defined Multinuclear Iridium-Aluminum Polyhydride Clusters and Comparative Reactivity. <i>Inorganic Chemistry</i> , 2022, 61, 5715-5730.	1.9	9
79	PMLABe Diol Synthesized by Ring-Opening Polymerization of Racemic Benzyl Malolactonate Initiated by Rare-Earth Trisborohydride Complexes: An Experimental and DFT Study. <i>Chemistry - A European Journal</i> , 2014, 20, 14387-14402.	1.7	8
80	Mechanistic Studies on the Catalytic Synthesis of BN Heterocycles (1,2,1-Benzazaboroles) at Ruthenium. <i>ACS Catalysis</i> , 2018, 8, 939-948.	5.5	8
81	Uncatalyzed Formation of Polyaminoboranes from Diisopropylaminoborane and Primary Amines: a Kinetically Controlled Polymerization Reaction. <i>Advanced Synthesis and Catalysis</i> , 2021, 363, 2417-2426.	2.1	8
82	Rationalizing the Reactivity of Mixed Allyl Rare-Earth Borohydride Complexes with DFT Studies. <i>Catalysts</i> , 2020, 10, 820.	1.6	7
83	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.	1.6	6
84	Nickel-catalyzed synthesis of Zn(i)-Zn(i) bonded compounds. <i>Chemical Communications</i> , 2021, 57, 13696-13699.	2.2	6
85	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.	1.9	5
86	Ruthenium Icosahedra and Ultrathin Platelets: The Role of Surface Chemistry on the Nanoparticle Structure. <i>Chemistry of Materials</i> , 2022, 34, 2931-2944.	3.2	5
87	Synthesis and Reactivity of Triangular Heterometallic Complexes Containing Zn-Zn Bond. <i>Inorganic Chemistry</i> , 2022, , .	1.9	5
88	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.	0.5	4
89	Alternative (1-N:1-6-arene vs. 2-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.	1.6	4
90	Speciation of [Cp* ₂ M ₂ O ₅] in Polar and Donor Solvents. <i>Chemistry - A European Journal</i> , 2013, 19, 3969-3985.	1.7	3

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91	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.	1.7	3
92	When organophosphorus ruthenium complexes covalently bind to ruthenium nanoparticles to form nanoscale hybrid materials. <i>Chemical Communications</i> , 2020, 56, 4059-4062.	2.2	3
93	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.	2.1	3
94	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.	0.5	2
95	How CuI and NaI Interact with Faujasite Zeolite? A Theoretical Investigation. <i>Journal of Physical Chemistry C</i> , 2020, 124, 28026-28037.	1.5	2
96	Molecular Thorium Trihydrido Clusters Stabilized by Cyclopentadienyl Ligands. <i>Angewandte Chemie</i> , 2020, 132, 11346-11351.	1.6	2
97	Supramolecular nanocapsules as two-fold stabilizers of outer-cavity sub-nanometric Ru NPs and inner-cavity ultra-small Ru clusters. <i>Nanoscale Horizons</i> , 2022, 7, 607-615.	4.1	2
98	Hydroboration of vinyl halides with mesitylborane: a direct access to (mesityl)(alkyl)haloboranes. <i>Chemical Communications</i> , 2022, 58, 1589-1592.	2.2	1
99	A Masked Form of an O^{B} -orylated Breslow Intermediate for the Diastereoselective FLP-type Activation of Aldehydes. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	1