# David Balcells

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 78 papers | 4,213 citations | 31 h-index | 64 g-index |
| 88 ext. papers | 4,557 ext. citations | 8.7 avg, IF | 5.59 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 78 | Computational Studies on the Mechanisms for Deaminative Amide Hydrogenation by Homogeneous Bifunctional Catalysts. *Topics in Catalysis*, **2022**, 65, 82-95 | 2.3 | 0 |
| 77 | Synthesis of Triarylmethanes via Palladium-Catalyzed Suzuki–Miyaura Reactions of Diarylmethyl Esters. *Organometallics*, **2021**, 40, 2332-2344 | 3.8 | 2 |
| 76 | Unsymmetrical Naphthyridine-Based Dicopper(I) Complexes: Synthesis, Stability, and Carbon–Hydrogen Bond Activations. *Organometallics*, **2021**, 40, 1866-1873 | 3.8 | 3 |
| 75 | C-H Activation by RuCoO Oxo Cubanes: Effects of Oxyl Radical Character and Metal-Metal Cooperativity. *Journal of the American Chemical Society*, **2021**, 143, 12108-12119 | 16.4 | 4 |
| 74 | Rational selection of co-catalysts for the deaminative hydrogenation of amides. *Chemical Science*, **2020**, 11, 2225-2230 | 9.4 | 8 |
| 73 | Machine learning dihydrogen activation in the chemical space surrounding Vaska's complex. *Chemical Science*, **2020**, 11, 4584-4601 | 9.4 | 47 |
| 72 | Concerted Proton-Electron Transfer Reactivity at a Multimetallic CoO Cubane Cluster. *Inorganic Chemistry*, **2020**, 59, 15553-15560 | 5.1 | 7 |
| 71 | First-Principles Calculation of H NMR Chemical Shifts of Complex Metal Polyhydrides: The Essential Inclusion of Relativity and Dynamics. *Inorganic Chemistry*, **2020**, 59, 17509-17518 | 5.1 | 3 |
| 70 | tmQM Dataset-Quantum Geometries and Properties of 86k Transition Metal Complexes. *Journal of Chemical Information and Modeling*, **2020**, 60, 6135-6146 | 6.1 | 21 |
| 69 | Synthesis, Characterization, and Reactivity of Cyclometalated Gold(III) Dihalide Complexes in Aqua Regia. *European Journal of Inorganic Chemistry*, **2020**, 2020, 3249-3258 | 2.3 | 3 |
| 68 | Bis(dialkylphosphino)ferrocene-Ligated Nickel(II) Precatalysts for Suzuki-Miyaura Reactions of Aryl Carbonates. *Organometallics*, **2019**, 38, 3377-3387 | 3.8 | 15 |
| 67 | Isolation and Study of Ruthenium-Cobalt Oxo Cubanes Bearing a High-Valent, Terminal Ru-Oxo with Significant Oxyl Radical Character. *Journal of the American Chemical Society*, **2019**, 141, 19859-19869 | 16.4 | 12 |
| 66 | A Career in Catalysis: Odile Eisenstein. *ACS Catalysis*, **2019**, 9, 10375-10388 | 13.1 | 1 |
| 65 | A DFT Perspective on Diels–Alder Organocatalysts Based on Substituted Phosphoramides. *European Journal of Organic Chemistry*, **2019**, 2019, 442-450 | 3.2 | 1 |
| 64 | Synthesis and Characterization of Stable Gold(III) PNP Pincer Complexes. *European Journal of Inorganic Chemistry*, **2018**, 2018, 3113-3117 | 2.3 | 6 |
| 63 | A Dinuclear Iridium(V,V) Oxo-Bridged Complex Characterized Using a Bulk Electrolysis Technique for Crystallizing Highly Oxidizing Compounds. *Inorganic Chemistry*, **2018**, 57, 5684-5691 | 5.1 | 12 |
| 62 | Cyclometalated ruthenium complexes with carboxylated ligands from a combined experimental/computational perspective. *Dalton Transactions*, **2018**, 47, 2589-2601 | 4.3 | 6 |

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| 61 | Designing Pd and Ni Catalysts for Cross-Coupling Reactions by Minimizing Off-Cycle Species. *ACS Catalysis*, **2018**, 8, 3499-3515 | 13.1 | 58 |
| 60 | Influence of a "Dangling" Co(II) Ion Bound to a [MnCoO] Oxo Cubane. *Journal of the American Chemical Society*, **2018**, 140, 9030-9033 | 16.4 | 18 |
| 59 | The Key Role of the Hemiaminal Intermediate in the Iron-Catalyzed Deaminative Hydrogenation of Amides. *ACS Catalysis*, **2018**, 8, 8751-8762 | 13.1 | 38 |
| 58 | 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 |
| 57 | The neutron diffraction structure of [Ir4(IMe)8H10]2+ polyhydride cluster: Testing the computational hydride positional assignments. *Journal of Organometallic Chemistry*, **2017**, 849-850, 17-21 | 2.3 | 6 |
| 56 | trans-Mutation at Gold(III): A Mechanistic Study of a Catalytic Acetylene Functionalization via a Double Insertion Pathway. *ACS Catalysis*, **2017**, 7, 5023-5034 | 13.1 | 28 |
| 55 | Quantum chemical modeling of the reaction path of chorismate mutase based on the experimental substrate/product complex. *FEBS Open Bio*, **2017**, 7, 789-797 | 2.7 | 7 |
| 54 | Mechanistic Study of an Improved Ni Precatalyst for Suzuki-Miyaura Reactions of Aryl Sulfamates: Understanding the Role of Ni(I) Species. *Journal of the American Chemical Society*, **2017**, 139, 922-936 | 16.4 | 102 |
| 53 | A competing, dual mechanism for catalytic direct benzene hydroxylation from combined experimental-DFT studies. *Chemical Science*, **2017**, 8, 8373-8383 | 9.4 | 19 |
| 52 | DFT Investigation of Suzuki-Miyaura Reactions with Aryl Sulfamates Using a Dialkylbiarylphosphine-Ligated Palladium Catalyst. *Organometallics*, **2017**, 36, 3664-3675 | 3.8 | 9 |
| 51 | Synthesis and Characterization of Iridium(V) Coordination Complexes With an N,O-Donor Organic Ligand. *Angewandte Chemie*, **2017**, 129, 13227-13231 | 3.6 | 7 |
| 50 | Synthesis and Characterization of Iridium(V) Coordination Complexes With an N,O-Donor Organic Ligand. *Angewandte Chemie - International Edition*, **2017**, 56, 13047-13051 | 16.4 | 15 |
| 49 | Redox Activity of Oxo-Bridged Iridium Dimers in an N,O-Donor Environment: Characterization of Remarkably Stable Ir(IV,V) Complexes. *Journal of the American Chemical Society*, **2017**, 139, 9672-9683 | 16.4 | 34 |
| 48 | Dinitrogen-Facilitated Reversible Formation of a Si□H Bond in a Pincer-Supported Ni Complex. *Organometallics*, **2016**, 35, 3154-3162 | 3.8 | 30 |
| 47 | Synthetic and Computational Studies on the Rhodium-Catalyzed Hydroamination of Aminoalkenes. *ACS Catalysis*, **2016**, 6, 5651-5665 | 13.1 | 15 |
| 46 | High Oxidation State Iridium Mono-□xo Dimers Related to Water Oxidation Catalysis. *Journal of the American Chemical Society*, **2016**, 138, 15917-15926 | 16.4 | 31 |
| 45 | Small-molecule activation at Au(iii): metallacycle construction from ethylene, water, and acetonitrile. *Dalton Transactions*, **2016**, 45, 14719-24 | 4.3 | 13 |
| 44 | Coordination and insertion of alkenes and alkynes in Au(III) complexes: nature of the intermediates from a computational perspective. *Dalton Transactions*, **2016**, 45, 5504-13 | 4.3 | 18 |

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| 43 | Deciphering Selectivity in Organic Reactions: A Multifaceted Problem. *Accounts of Chemical Research*, **2016**, 49, 1070-8 | 24.3 | 25 |
| 42 | Design of a Versatile and Improved Precatalyst Scaffold for Palladium-Catalyzed Cross-Coupling: (η3-1-tBu-indenyl)2(μ-Cl)2Pd2. *ACS Catalysis*, **2015**, 5, 3680-3688 | 13.1 | 101 |
| 41 | Gel-assisted crystallization of [Ir4(IMe)7(CO)H10](2+) and [Ir4(IMe)8H9](3+) clusters derived from catalytic glycerol dehydrogenation. *Dalton Transactions*, **2015**, 44, 18403-10 | 4.3 | 18 |
| 40 | Understanding Precatalyst Activation in Cross-Coupling Reactions: Alcohol Facilitated Reduction from Pd(II) to Pd(0) in Precatalysts of the Type (η3-allyl)Pd(L)(Cl) and (η3-indenyl)Pd(L)(Cl). *ACS Catalysis*, **2015**, 5, 5596-5606 | 13.1 | 76 |
| 39 | Understanding the Solution and Solid-State Structures of Pd and Pt PSiP Pincer-Supported Hydrides. *Inorganic Chemistry*, **2015**, 54, 11411-22 | 5.1 | 23 |
| 38 | Effect of 2-Substituents on Allyl-Supported Precatalysts for the Suzuki–Miyaura Reaction: Relating Catalytic Efficiency to the Stability of Palladium(I) Bridging Allyl Dimers. *Organometallics*, **2015**, 34, 381-394 | 3.8 | 33 |
| 37 | Nickel(I) monomers and dimers with cyclopentadienyl and indenyl ligands. *Chemistry - A European Journal*, **2014**, 20, 5327-37 | 4.8 | 57 |
| 36 | Does the metal protect the ancillary ligands? C-H strengthening and deactivation in amines and phosphines upon metal-binding. *Chemical Communications*, **2014**, 50, 614-6 | 5.8 | 16 |
| 35 | Conformational complexity of morphine and morphinum in the gas phase and in water. A DFT and MP2 study. *RSC Advances*, **2014**, 4, 24729-24735 | 3.7 | 0 |
| 34 | Experimental and computational studies of borohydride catalyzed hydrosilylation of a variety of CO and CN functionalities including esters, amides and heteroarenes. *New Journal of Chemistry*, **2014**, 38, 1694-1700 | 3.6 | 34 |
| 33 | Insight into the efficiency of cinnamyl-supported precatalysts for the Suzuki-Miyaura reaction: observation of Pd(I) dimers with bridging allyl ligands during catalysis. *Journal of the American Chemical Society*, **2014**, 136, 7300-16 | 16.4 | 102 |
| 32 | Distortional Effects of Noncovalent Interactions in the Crystal Lattice of a Cp*Ir(III) Acylhydroxamic Acid Complex: A Joint Experimental–Computational Study. *Organometallics*, **2014**, 33, 4417-4424 | 3.8 | 1 |
| 31 | A carbene-rich but carbonyl-poor [Ir6 (IMe)8 (CO)2 H14 ](2+) polyhydride cluster as a deactivation product from catalytic glycerol dehydrogenation. *Angewandte Chemie - International Edition*, **2014**, 53, 12808-11 | 16.4 | 37 |
| 30 | A Carbene-Rich but Carbonyl-Poor [Ir6(IMe)8(CO)2H14]2+ Polyhydride Cluster as a Deactivation Product from Catalytic Glycerol Dehydrogenation. *Angewandte Chemie*, **2014**, 126, 13022-13025 | 3.6 | 9 |
| 29 | Generation and Structural Characterization of a Gold(III) Alkene Complex. *Angewandte Chemie*, **2013**, 125, 1704-1707 | 3.6 | 24 |
| 28 | Introducing copper as catalyst for oxidative alkane dehydrogenation. *Journal of the American Chemical Society*, **2013**, 135, 3887-96 | 16.4 | 66 |
| 27 | Generation and structural characterization of a gold(III) alkene complex. *Angewandte Chemie - International Edition*, **2013**, 52, 1660-3 | 16.4 | 56 |
| 26 | Cp* Iridium Precatalysts for Selective C–H Oxidation via Direct Oxygen Insertion: A Joint Experimental/Computational Study. *ACS Catalysis*, **2012**, 2, 208-218 | 13.1 | 78 |

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| 25 | Basic ancillary ligands promote O-O bond formation in iridium-catalyzed water oxidation: a DFT study. *Dalton Transactions*, **2011**, 40, 11241-7 | 4.3 | 40 |
| 24 | Half-sandwich iridium complexes for homogeneous water-oxidation catalysis. *Journal of the American Chemical Society*, **2010**, 132, 16017-29 | 16.4 | 468 |
| 23 | An Experimental−Theoretical Study of the Factors That Affect the Switch between Ruthenium-Catalyzed Dehydrogenative Amide Formation versus Amine Alkylation. *Organometallics*, **2010**, 29, 6548-6558 | 3.8 | 98 |
| 22 | C-H bond activation in transition metal species from a computational perspective. *Chemical Reviews* , **2010**, 110, 749-823 | 68.1 | 877 |
| 21 | Manganese catalysts for C-H activation: an experimental/theoretical study identifies the stereoelectronic factor that controls the switch between hydroxylation and desaturation pathways. *Journal of the American Chemical Society*, **2010**, 132, 7605-16 | 16.4 | 94 |
| 20 | Highly active and robust Cp* iridium complexes for catalytic water oxidation. *Journal of the American Chemical Society*, **2009**, 131, 8730-1 | 16.4 | 516 |
| 19 | Molecular recognition in Mn-catalyzed C-H oxidation. Reaction mechanism and origin of selectivity from a DFT perspective. *Dalton Transactions*, **2009**, 5989-6000 | 4.3 | 25 |
| 18 | C-H oxidation by hydroxo manganese(v) porphyrins: a DFT study. *Chemical Communications*, **2009**, 1772-4 | 5.8 | 41 |
| 17 | Mechanism of Homogeneous Iridium-Catalyzed Alkylation of Amines with Alcohols from a DFT Study. *Organometallics*, **2008**, 27, 2529-2535 | 3.8 | 142 |
| 16 | The rebound mechanism in catalytic C-H oxidation by MnO(tpp)Cl from DFT studies: electronic nature of the active species. *Chemical Communications*, **2008**, 744-6 | 5.8 | 64 |
| 15 | A rational basis for the axial ligand effect in C-H oxidation by [MnO(porphyrin)(X)]+ (X = H2O, OH-, O2-) from a DFT study. *Inorganic Chemistry*, **2008**, 47, 10090-9 | 5.1 | 84 |
| 14 | Atom economic synthesis of amidesvia transition metal catalyzed rearrangement of oxaziridines. *Green Chemistry*, **2007**, 9, 976 | 10 | 31 |
| 13 | Computational approaches to asymmetric synthesis. *New Journal of Chemistry*, **2007**, 31, 333 | 3.6 | 99 |
| 12 | How does the Achiral Base Decide the Stereochemical Outcome in the Dynamic Kinetic Resolution of Sulfinyl Chlorides? A Computational Study. *Advanced Synthesis and Catalysis*, **2007**, 349, 2103-2110 | 5.6 | 16 |
| 11 | Mechanism of the base-assisted displacement of chloride by alcohol in sulfinyl derivatives. *Journal of Organic Chemistry*, **2006**, 71, 6388-96 | 4.2 | 39 |
| 10 | Computational rationalization of the dependence of the enantioselectivity on the nature of the catalyst in the vanadium-catalyzed oxidation of sulfides by hydrogen peroxide. *Journal of the American Chemical Society*, **2005**, 127, 3624-34 | 16.4 | 68 |
| 9 | Base-catalyzed inversion of chiral sulfur centers. A computational study. *Organic Letters*, **2004**, 6, 2197-200 | 6.2 | 18 |
| 8 | Self-Consistency versus "Best-Fit" Approaches in Understanding the Structure of Metal Nitrosyl Complexes. *Organometallics*, **2004**, 23, 6008-6014 | 3.8 | 4 |

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| 7 | Polyene Cyclization by a Double Intramolecular Heck Reaction. A DFT Study. *Organometallics*, **2004**, 23, 2784-2796 | 3.8 | 31 |
| 6 | Some critical issues in the application of quantum mechanics/molecular mechanics methods to the study of transition metal complexes. *Faraday Discussions*, **2003**, 124, 429-41; discussion 443-55 | 3.6 | 25 |
| 5 | Density functional study on the mechanism of the vanadium-catalyzed oxidation of sulfides by hydrogen peroxide. *Journal of Organic Chemistry*, **2003**, 68, 4265-74 | 4.2 | 55 |
| 4 | An oscillating C2(2-) unit inside a copper rectangle. *Chemical Communications*, **2003**, 1260-1 | 5.8 | 15 |
| 3 | Computational Studies on Asymmetric Reactions with Sulfur Reagents399-416 | | 0 |
| 2 | Automated Construction and Optimization Combined with Machine Learning to Generate Pt(II) Methane C H Activation Transition States. *Topics in Catalysis*,1 | 2.3 | 1 |
| 1 | Concerted Cycloaddition Mechanism in the CuAAC Reaction Catalyzed by 1,8-Naphthyridine Dicopper Complexes. *ACS Catalysis*,4744-4753 | 13.1 | 0 |