Feliu Maseras

List of Publications by Citations

285 papers	14,621 citations	60 h-index	108 g-index
315 ext. papers	15,655 ext. citations	7.5 avg, IF	6.71 L-index

#	Paper	IF	Citations
285	IMOMM: A new integrated ab initio + molecular mechanics geometry optimization scheme of equilibrium structures and transition states. *Journal of Computational Chemistry*, **1995**, 16, 1170-1179	3.5	1464
284	Proton abstraction mechanism for the palladium-catalyzed intramolecular arylation. *Journal of the American Chemical Society*, **2006**, 128, 1066-7	16.4	643
283	Proton-abstraction mechanism in the palladium-catalyzed intramolecular arylation: substituent effects. *Journal of the American Chemical Society*, **2007**, 129, 6880-6	16.4	479
282	Direct arylation of arene C-H bonds by cooperative action of NHcarbene-ruthenium(II) catalyst and carbonate via proton abstraction mechanism. *Journal of the American Chemical Society*, **2008**, 130, 1156-7	16.4	347
281	A DFT Study of the Full Catalytic Cycle of the Suzuki Miyaura Cross-Coupling on a Model System. *Organometallics*, **2006**, 25, 3647-3658	3.8	324
280	Transition metal polyhydrides: from qualitative ideas to reliable computational studies. *Chemical Reviews*, **2000**, 100, 601-36	68.1	304
279	Managing the computational chemistry big data problem: the ioChem-BD platform. *Journal of Chemical Information and Modeling*, **2015**, 55, 95-103	6.1	289
278	Computational characterization of the role of the base in the Suzuki-Miyaura cross-coupling reaction. *Journal of the American Chemical Society*, **2005**, 127, 9298-307	16.4	284
277	Computational perspective on Pd-catalyzed C-C cross-coupling reaction mechanisms. *Accounts of Chemical Research*, **2013**, 46, 2626-34	24.3	253
276	Merging sustainability with organocatalysis in the formation of organic carbonates by using CO(2) as a feedstock. *ChemSusChem*, **2012**, 5, 2032-8	8.3	247
275	Redox Non-innocent Ligand Controls Water Oxidation Overpotential in a New Family of Mononuclear Cu-Based Efficient Catalysts. *Journal of the American Chemical Society*, **2015**, 137, 6758-61	16.4	210
274	[(NHC)AuI]-catalyzed formation of conjugated enones and enals: an experimental and computational study. *Chemistry - A European Journal*, **2007**, 13, 6437-51	4.8	168
273	C-C reductive elimination in palladium complexes, and the role of coupling additives. A DFT study supported by experiment. *Journal of the American Chemical Society*, **2009**, 131, 3650-7	16.4	167
272	A valuable, inexpensive Cui/n-heterocyclic carbene catalyst for the selective diboration of styrene. *Chemistry - A European Journal*, **2007**, 13, 2614-21	4.8	145
271	Experimental and theoretical investigations of new dinuclear palladium complexes as precatalysts for the amination of aryl chlorides. *Journal of the American Chemical Society*, **2006**, 128, 6376-90	16.4	141
270	A general mechanism for the copper- and silver-catalyzed olefin aziridination reactions: concomitant involvement of the singlet and triplet pathways. *Journal of the American Chemical Society*, **2013**, 135, 1338-48	16.4	136
269	Metal-arene interactions in dialkylbiarylphosphane complexes of copper, silver, and gold. *Chemistry - A European Journal*, **2010**, 16, 5324-32	4.8	135

268	Catecholborane Bound to Titanocene. Unusual Coordination of Ligand Bonds. *Journal of the American Chemical Society*, **1996**, 118, 10936-10937	16.4	133
267	Application of the New Integrated MO + MM (IMOMM) Method to the Organometallic Reaction Pt(PR3)2 + H2 (R = H, Me, t-Bu, and Ph). *The Journal of Physical Chemistry*, **1996**, 100, 2573-2580		130
266	Unraveling the origin of regioselectivity in rhodium diphosphine catalyzed hydroformylation. A DFT QM/MM study. *Journal of the American Chemical Society*, **2001**, 123, 7630-7	16.4	127
265	Computational study of the transmetalation process in the Suzuki Miyaura cross-coupling of aryls. *Journal of Organometallic Chemistry*, **2006**, 691, 4459-4466	2.3	122
264	Catalytic Mechanism of Galactose Oxidase: A Theoretical Study. *Journal of the American Chemical Society*, **2000**, 122, 8031-8036	16.4	117
263	Bidentate phosphines as ligands in the palladium-catalyzed intramolecular arylation: the intermolecular base-assisted proton abstraction mechanism. *Tetrahedron*, **2008**, 64, 6021-6029	2.4	115
262	Gold(I)-catalyzed intermolecular hydroalkoxylation of allenes: a DFT study. *Organic Letters*, **2009**, 11, 2237-40	6.2	114
261	Selective homogeneous and heterogeneous gold catalysis with alkynes and alkenes: similar behavior, different origin. *ChemPhysChem*, **2008**, 9, 1624-9	3.2	111
260	Stereoselective and Versatile Preparation of Tri- and Tetrasubstituted Allylic Amine Scaffolds under Mild Conditions. *Journal of the American Chemical Society*, **2016**, 138, 11970-8	16.4	109
259	Computational Evidence of the Importance of Substituent Bulk on Agostic Interactions in Ir(H)2(PtBu2Ph)2+. *Journal of the American Chemical Society*, **1998**, 120, 361-365	16.4	106
258	Theory Does Not Support an Osmaoxetane Intermediate in the Osmium-Catalyzed Dihydroxylation of Olefins. *Journal of the American Chemical Society*, **1996**, 118, 11660-11661	16.4	104
257	Computational approaches to asymmetric synthesis. *New Journal of Chemistry*, **2007**, 31, 333	3.6	99
256	Protonation of transition-metal hydrides: a not so simple process. *Chemical Society Reviews*, **2009**, 38, 957-66	58.5	93
255	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, 14571-8	16.4	93
254	Computational and Experimental Test of Steric Influence on Agostic Interactions: A Homologous Series for Ir(III). *Journal of the American Chemical Society*, **1999**, 121, 97-106	16.4	92
253	Scope and Challenge of Computational Methods for Studying Mechanism and Reactivity in Homogeneous Catalysis. *ACS Catalysis*, **2019**, 9, 6803-6813	13.1	91
252	A Domino Process toward Functionally Dense Quaternary Carbons through Pd-Catalyzed Decarboxylative C(sp)-C(sp) Bond Formation. *Journal of the American Chemical Society*, **2018**, 140, 3981-3987	16.4	87
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250	Reactions of a Hexahydride Osmium Complex with Aromatic Ketones: C–H Activation versus C–H Activations. *Organometallics*, **2001**, 20, 442-452	3.8	85
249	Mechanism of the gold-catalyzed cyclopropanation of alkenes with 1,6-enynes. *Chemical Science*, **2011**, 2, 141-149	9.4	83
248	Inertness of the Aryl–H Bond toward Oxidative Addition to Osmium and Rhodium Complexes: Thermodynamic or Kinetic Origin?. *Journal of the American Chemical Society*, **1998**, 120, 12634-12640	16.4	83
247	Calculation of Reaction Free Energies in Solution: A Comparison of Current Approaches. *Journal of Physical Chemistry A*, **2018**, 122, 1392-1399	2.8	82
246	Theoretical Study on the Origin of Enantioselectivity in the Bis(dihydroquinidine)-3,6-pyridazine Osmium Tetroxide-Catalyzed Dihydroxylation of Styrene. *Journal of the American Chemical Society*, **1999**, 121, 1317-1323	16.4	82
245	Transition metal catalysis by density functional theory and density functional theory/molecular mechanics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 375-385	7.9	78
244	Application of the natural population analysis to transition-metal complexes. Should the empty metal p orbitals be included in the valence space?. *Chemical Physics Letters*, **1992**, 195, 500-504	2.5	77
243	Chemo-, regio-, and stereoselective silver-catalyzed aziridination of dienes: scope, mechanistic studies, and ring-opening reactions. *Journal of the American Chemical Society*, **2014**, 136, 5342-50	16.4	76
242	Mechanism of Alkane C–H Bond Activation by Copper and Silver Homoscorpionate Complexes. *Organometallics*, **2006**, 25, 5292-5300	3.8	74
241	practical implications of boron-to-zinc transmetalation for the catalytic asymmetric arylation of aldehydes. *Angewandte Chemie - International Edition*, **2008**, 47, 1098-101	16.4	71
240	Palladium round trip in the Negishi coupling of trans-[PdMeCl(PMePh2)2] with ZnMeCl: an experimental and DFT study of the transmetalation step. *Chemistry - A European Journal*, **2010**, 16, 8596-9	4.8	70
239	Brønsted acid catalyzed Morita-Baylis-Hillman reaction: a new mechanistic view for thioureas revealed by ESI-MS(/MS) monitoring and DFT calculations. *Chemistry - A European Journal*, **2009**, 15, 12460-9	4.8	69
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235	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
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227	Competitive and selective Csp3-Br versus Csp2-Br bond activation in palladium-catalysed Suzuki cross-coupling: an experimental and theoretical study of the role of phosphine ligands. *Chemistry - A European Journal*, **2010**, 16, 13390-7	4.8	62
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225	Microkinetic modeling in homogeneous catalysis. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1372	7.9	60
224	Rationale for the sluggish oxidative addition of aryl halides to Au(I). *Chemical Communications*, **2014**, 50, 1533-6	5.8	59
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221	Amine conformational change and spin conversion induced by metal-assisted ligand oxidation: from the seven-coordinate iron(II)–PAA complex to the two oxidized iron(II)(bpy)3tren isomers. Characterization, crystal structures, and density functional study. *Inorganica Chimica Acta*, **2000**, 297, 338-350	2.7	57
220	Oxidative Coupling Mechanisms: Current State of Understanding. *ACS Catalysis*, **2018**, 8, 1161-1172	13.1	56
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214	Cyclobutene vs 1,3-Diene Formation in the Gold-Catalyzed Reaction of Alkynes with Alkenes: The Complete Mechanistic Picture. *Journal of the American Chemical Society*, **2017**, 139, 10302-10311	16.4	52
213	A DFT Study of the Effect of the Ligands in the Reductive Elimination from Palladium Bis(allyl) Complexes *Organometallics*, **2010**, 29, 4983-4991	3.8	52
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208	A theoretical analysis of a classic example of supramolecular catalysis. *Chemical Communications*, **2007**, 748-50	5.8	50
207	Crucial role of anions on the deprotonation of the cationic dihydrogen complex trans-[FeH(eta2-H2)(dppe)2]+. *Journal of the American Chemical Society*, **2007**, 129, 6608-18	16.4	50
206	Hydride Exchange Processes in the Coordination Sphere of Transition Metal Complexes: The OsH3(BH4)(PR3)2 System. *Journal of the American Chemical Society*, **1996**, 118, 8388-8394	16.4	50
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201	Toward a mechanistic understanding of oxidative homocoupling: the Glaser Hay reaction. *Catalysis Science and Technology*, **2014**, 4, 4200-4209	5.5	46
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190	Light-Driven Enantioselective Organocatalytic Benzylation of Enals. *Angewandte Chemie - International Edition*, **2017**, 56, 3304-3308	16.4	43
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183	Mechanistic Studies on Gold-Catalyzed Direct Arene CH Bond Functionalization by Carbene Insertion: The Coinage-Metal Effect. *Organometallics*, **2017**, 36, 172-179	3.8	41
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177	Mechanism of the base-assisted displacement of chloride by alcohol in sulfinyl derivatives. *Journal of Organic Chemistry*, **2006**, 71, 6388-96	4.2	39
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174	Cooperative Reductive Elimination: The Missing Piece in the Oxidative-Coupling Mechanistic Puzzle. *Angewandte Chemie - International Edition*, **2016**, 55, 2764-7	16.4	38
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166	C-H bond activation of benzene by unsaturated η2-cyclopropene and η2-benzyne complexes of niobium. *Journal of the American Chemical Society*, **2010**, 132, 14239-50	16.4	35
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153	Site Preference Energetics, Fluxionality, and Intramolecular M□□□H□□N Hydrogen Bonding in a Dodecahedral Transition Metal Polyhydride□ *Inorganic Chemistry*, **1997**, 36, 5505-5511	5.1	30
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