Xavier Solans-Monfort

List of Publications by Year
in descending order

68	2,713	172457	182427
papers	citations	29 h-index	51 g-index

71	71	71	2303
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Understanding d0-Olefin Metathesis Catalysts:Â Which Metal, Which Ligands?. Journal of the American Chemical Society, 2007, 129, 8207-8216.	13.7	210
2	Dinitrogen Dissociation on an Isolated Surface Tantalum Atom. Science, 2007, 317, 1056-1060.	12.6	163
3	d0Re-Based Olefin Metathesis Catalysts, Re(â‹®CR)(CHR)(X)(Y):Â The Key Role of X and Y Ligands for Efficient Active Sites. Journal of the American Chemical Society, 2005, 127, 14015-14025.	13.7	158
4	A Well-Defined, Silica-Supported Tungsten Imido Alkylidene Olefin Metathesis Catalyst. Organometallics, 2006, 25, 3554-3557.	2.3	152
5	Shutting Down Secondary Reaction Pathways: The Essential Role of the Pyrrolyl Ligand in Improving Silica Supported d⁰-ML₄ Alkene Metathesis Catalysts from DFT Calculations. Journal of the American Chemical Society, 2010, 132, 7750-7757.	13.7	121
6	Dynamics of Silica-Supported Catalysts Determined by Combining Solid-State NMR Spectroscopy and DFT Calculations. Journal of the American Chemical Society, 2008, 130, 5886-5900.	13.7	98
7	Adsorption of NH3and H2O in Acidic Chabazite. Comparison of ONIOM Approach with Periodic Calculations. Journal of Physical Chemistry B, 2005, 109, 3539-3545.	2.6	96
8	Can Cu+-Exchanged Zeolites Store Molecular Hydrogen? An Ab-Initio Periodic Study Compared with Low-Temperature FTIR. Journal of Physical Chemistry B, 2004, 108, 8278-8286.	2.6	91
9	Î²-H Transfer from the Metallacyclobutane: A Key Step in the Deactivation and Byproduct Formation for the Well-Defined Silica-Supported Rhenium Alkylidene Alkene Metathesis Catalyst. Journal of the American Chemical Society, 2008, 130, 6288-6297.	13.7	88
10	Differences in the Activation Processes of Phosphine-Containing and Grubbsâ€“Hoveyda-Type Alkene Metathesis Catalysts. Organometallics, 2012, 31, 4203-4215.	2.3	85
11	Oxo vs Imido Alkylidene d⁰-Metal Species: How and Why Do They Differ in Structure, Activity, and Efficiency in Alkene Metathesis?. Organometallics, 2012, 31, 6812-6822.	2.3	81
12	DFT Mechanistic Study on Diene Metathesis Catalyzed by Ruâ€Based Grubbsâ€“Hoveydaâ€Type Carbenes: The Key Role of Ï€â€Electron Density Delocalization in the Hoveyda Ligand. Chemistry - A European Journal, 2010, 16, 7331-7343.	3.3	78
13	Structure, spectroscopic and electronic properties of a well defined silica supported olefin metathesis catalyst, [(î€,SiO)Re(î€,CR)(î€CHR)(CH2R)], through DFT periodic calculations: silica is just a large siloxy ligand. New Journal of Chemistry, 2006, 30, 842-850.	2.8	77
14	Understanding Structural and Dynamic Properties of Well-Defined Rhenium-Based Olefin Metathesis Catalysts, Re(â‹®CR)(CHR)(X)(Y), from DFT and QM/MM Calculations. Organometallics, 2005, 24, 1586-1597.	2.3	59
15	DFT calculations of d0M(NR)(CHtBu)(X)(Y) (M = Mo, W; R = CPh3, 2,6-iPrâ€“C6H3; X and Y = CH2tBu, OtBu,) Tj ETQq1 1 0.784314 rgB Transactions, 2006, , 3077-3087.	3.3	58
16	Mechanistic Insights into Ringâ€Closing Enyne Metathesis with the Secondâ€Generation Grubbsâ€“Hoveyda Catalyst: A DFT Study. Chemistry - A European Journal, 2011, 17, 7506-7520.	3.3	56
17	Metallacyclobutanes from Schrock-Type d⁰ Metal Alkylidene Catalysts: Structural Preferences and Consequences in Alkene Metathesis. Organometallics, 2015, 34, 1668-1680.	2.3	55
18	Electron hole formation in acidic zeolite catalysts. Journal of Chemical Physics, 2004, 121, 6034-6041.	3.0	49

#	Article	IF	Citations
19	Visibleâ€Light Photocatalytic Intramolecular Cyclopropane Ring Expansion. Angewandte Chemie - International Edition, 2017, 56, 7826-7830.	13.8	47
20	Atomically Dispersed Iridium on Indium Tin Oxide Efficiently Catalyzes Water Oxidation. ACS Central Science, 2020, 6, 1189-1198.	11.3	47
21	Ketoâ^'Enol Isomerization of Acetaldehyde in HZSM5. A Theoretical Study Using the ONIOM2 Method. Journal of Physical Chemistry B, 2002, 106, 10220-10226.	2.6	46
22	DFT calculations of NMR JCâ€“H coupling constants: An additional tool to characterize the Î±-agostic interaction in high oxidation state M-alkylidene complexes (M=Re, Mo and Ta). Polyhedron, 2006, 25, 339-348.	2.2	35
23	Successive Heterolytic Cleavages of H₂ Achieve N₂ Splitting on Silica-Supported Tantalum Hydrides: A DFT Proposed Mechanism. Inorganic Chemistry, 2012, 51, 7237-7249.	4.0	35
24	Binding of Thioflavin T and Related Probes to Polymorphic Models of Amyloid-Î² Fibrils. Journal of Physical Chemistry B, 2017, 121, 8926-8934.	2.6	34
25	Toward Olefin Metathesis with Iron Carbene Complexes: Benefits of Tridentate Ïƒ-Donating Ligands. Organometallics, 2016, 35, 3914-3923.	2.3	32
26	Exo/endo Selectivity of the Ring-Closing Enyne Methathesis Catalyzed by Second Generation Ru-Based Catalysts. Influence of Reactant Substituents. ACS Catalysis, 2013, 3, 206-218.	11.2	31
27	DFT Study on the Relative Stabilities of Substituted Ruthenacyclobutane Intermediates Involved in Olefin Cross-Metathesis Reactions and Their Interconversion Pathways. Organometallics, 2014, 33, 6065-6075.	2.3	31
28	Spin-forbidden N2O dissociation in Cuâ€“ZSM-5. Chemical Physics Letters, 2003, 368, 242-246.	2.6	30
29	DFT Study on the Recovery of Hoveydaâ€“Grubbsâ€Type Catalyst Precursors in Enyne and Diene Ringâ€Closing Metathesis. Chemistry - A European Journal, 2013, 19, 14553-14565.	3.3	30
30	Water Adsorption on MO₂ (M = Ti, Ru, and Ir) Surfaces. Importance of Octahedral Distortion and Cooperative Effects. ACS Omega, 2019, 4, 2989-2999.	3.5	28
31	Periodic DFT Study of Radical Species on Crystalline Silica Surfaces. Journal of Physical Chemistry C, 2010, 114, 16430-16438.	3.1	27
32	Reactivity of Metal Carbenes with Olefins: Theoretical Insights on the Carbene Electronic Structure and Cyclopropanation Reaction Mechanism. Journal of Physical Chemistry A, 2018, 122, 1702-1712.	2.5	26
33	Theoretical Study of the Structure of ZCu(NO2)(NO). A Proposed Intermediate in the NOx Decomposition by Cuâ^'ZSM-5. Journal of Physical Chemistry A, 2000, 104, 3225-3230.	2.5	25
34	On the NO Decomposition by Cuâ^'ZSM-5 through the ZCu(NO2)(NO) or ZCu(N2O3) Intermediates. Journal of Physical Chemistry B, 2002, 106, 1372-1379.	2.6	25
35	Disaggregation-induced fluorescence enhancement of NIAD-4 for the optical imaging of amyloid-Î² fibrils. Physical Chemistry Chemical Physics, 2015, 17, 19718-19725.	2.8	24
36	Hydrogen Bond vs Proton Transfer in HZSM5 Zeolite. A Theoretical Study. Journal of Physical Chemistry B, 2005, 109, 19301-19308.	2.6	22

#	Article	IF	Citations
37	On the electronic structure of second generation Hoveydaâ€“Grubbs alkene metathesis precursors. Computational and Theoretical Chemistry, 2012, 996, 57-67.	2.5	21
38	Origin of the Enhanced Interaction of Molecular Hydrogen with Extraframework Cu⁺ and FeO⁺ Cations in Zeolite Hosts. A Periodic DFT Study. Journal of Physical Chemistry C, 2010, 114, 13926-13934.	3.1	20
39	A DFT periodic study on the interaction between O₂and cation exchanged chabazite MCHA (M = H+, Na+ or Cu+): effects in the tripletâ€“singlet energy gap. Physical Chemistry Chemical Physics, 2010, 12, 442-452.	2.8	19
40	DFT study on the reaction mechanism of the ring closing enyne metathesis (RCEYM) catalyzed by molybdenum alkylidene complexes. Dalton Transactions, 2014, 43, 4573-4586.	3.3	18
41	Interaction between Ruthenium Oxide Surfaces and Water Molecules. Effect of Surface Morphology and Water Coverage. Journal of Physical Chemistry C, 2019, 123, 7786-7798.	3.1	18
42	Importance of the oxyl character on the IrO2 surface dependent catalytic activity for the oxygen evolution reaction. Journal of Catalysis, 2021, 396, 192-201.	6.2	18
43	Organocatalytic vs. Ru-based electrochemical hydrogenation of nitrobenzene in competition with the hydrogen evolution reaction. Dalton Transactions, 2020, 49, 6446-6456.	3.3	17
44	Metal fragment isomerisation upon grafting a d2 ML4 perhydrocarbyl Os complex on a silica surface: origin and consequence. Dalton Transactions, 2009, , 5879.	3.3	16
45	Oâ€“O Bond activation in H2O2 and (CH3)3C-OOH mediated by [Ni(cyclam)(CH3CN)2](ClO4)2: Different mechanisms to form the same Ni(iii) product?. Dalton Transactions, 2011, 40, 6868.	3.3	15
46	H/D Exchange on Silica-Grafted Tantalum(V) Imido Amido [(â‰¡SiO)2Ta(V)(NH)(NH2)] Synthesized from Either Ammonia or Dinitrogen: IR and DFT Evidence for Heterolytic Splitting of D2. Topics in Catalysis, 2009, 52, 1482-1491.	2.8	14
47	Mechanistic Insights into Alkane Metathesis Catalyzed by Silica-Supported Tantalum Hydrides: A DFT Study. Inorganic Chemistry, 2017, 56, 10458-10473.	4.0	14
48	Influence of Ligands and Oxidation State on the Reactivity of Pentacoordinated Iron Carbenes with Olefins: Metathesis versus Cyclopropanation. Organometallics, 2018, 37, 1229-1241.	2.3	14
49	BCN-M: A Free Computational Tool for Generating Wulff-like Nanoparticle Models with Controlled Stoichiometry. Journal of Physical Chemistry C, 2020, 124, 1227-1237.	3.1	13
50	Metal coordination determines the catalytic activity of IrO2 nanoparticles for the oxygen evolution reaction. Journal of Catalysis, 2022, 412, 78-86.	6.2	13
51	Basic and acidic bifunctional catalysis: application to the tautomeric equilibrium of formamide. Chemical Physics, 2003, 295, 151-158.	1.9	12
52	Coordination of NO2to Cu and Mg in M(NO2)2Complexes. A Theoretical Study. Inorganic Chemistry, 1998, 37, 4512-4517.	4.0	11
53	Influence of Ï€-stacking on the N7 and O6 proton affinity of guanine. Theoretical Chemistry Accounts, 2009, 123, 105-111.	1.4	11
54	Heterolytic cleavage of ammonia Nâ€“H bond by bifunctional activation in silica-grafted single site Ta(V) imido amido surface complex. Importance of the outer sphere NH3 assistance. New Journal of Chemistry, 2011, 35, 1011.	2.8	11

#	Article	IF	Citations
55	Enhanced photocatalytic activity of gold nanoparticles driven by supramolecular hostâ€“guest chemistry. Chemical Communications, 2017, 53, 2126-2129.	4.1	11
56	Synthesis of Vanadium Oxo Alkylidene Complex and Its Reactivity in Ring-Closing Olefin Metathesis Reactions. Organometallics, 2021, 40, 2939-2944.	2.3	11
57	Switching acidic and basic catalysis through supramolecular functionalization in a porous 3D covalent imine-based material. Catalysis Science and Technology, 2019, 9, 6007-6014.	4.1	10
58	Computational study on donorâ€“acceptor optical markers for Alzheimer's disease: a game of charge transfer and electron delocalization. Physical Chemistry Chemical Physics, 2016, 18, 11634-11643.	2.8	9
59	Vanadium Imido NHC Complexes for Ring-Closing Olefin Metathesis Reactions. Organometallics, 2022, 41, 361-365.	2.3	9
60	Hydrazine Nâ€“N Bond Cleavage over Silica-Supported Tantalum-Hydrides. Inorganic Chemistry, 2015, 54, 11648-11659.	4.0	8
61	Surface morphology controls water dissociation on hydrated IrO₂ nanoparticles. Nanoscale, 2021, 13, 14480-14489.	5.6	8
62	Controlling the Formation of Two Concomitant Polymorphs in Hg(II) Coordination Polymers. Inorganic Chemistry, 2022, 61, 4965-4979.	4.0	7
63	Influence of Aromatic Cations on the Structural Arrangement of Hg(II) Halides. ACS Omega, 2020, 5, 29357-29372.	3.5	3
64	Effect of Lewis Acids on the Catalyst Activity for Alkene Metathesis, Z-/E- Selectivity and Stability of Tungsten Oxo Alkylidenes. Topics in Catalysis, 2022, 65, 433-447.	2.8	3
65	The role of charge transfer in the photophysics of dithiophene-based (NIADs) fluorescent markers for amyloid-Î² detection. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	2
66	Fluorescent Markers for Amyloidâ€Î² Detection: Computational Insights. Israel Journal of Chemistry, 2017, 57, 686-698.	2.3	2
67	A Hg(<scp>i</scp>) corrugated sheet assembled by auxiliary dioxole groups and Hgâ‹¯Ï€ interactions. CrystEngComm, 2022, 24, 4351-4355.	2.6	1
68	Can Cu+-Exchanged Zeolites Store Molecular Hydrogen? An ab initio Periodic Study Compared with Low-Temperature FTIR.. ChemInform, 2004, 35, no.	0.0	0