

Salvador Moncho

List of Publications by Year in descending order

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51
papers

1,022
citations

394286

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all docs

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docs citations

51
times ranked

1587
citing authors

#	ARTICLE	IF	CITATIONS
1	ZIF-67 Framework: A Promising New Candidate for Propylene/Propane Separation. Experimental Data and Molecular Simulations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 8116-8124.	1.5	121
2	Molecular Simulation Studies of the Diffusion of Methane, Ethane, Propane, and Propylene in ZIF-8. <i>Journal of Physical Chemistry C</i> , 2015, 119, 27028-27037.	1.5	94
3	Relativistic Zeroth-Order Regular Approximation Combined with Nonhybrid and Hybrid Density Functional Theory: Performance for NMR Indirect Nuclear Spin-Spin Coupling in Heavy Metal Compounds. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 223-234.	2.3	62
4	Ring opening metathesis polymerization (ROMP) of five- to eight-membered cyclic olefins: Computational, thermodynamic, and experimental approach. <i>Journal of Polymer Science Part A</i> , 2017, 55, 3137-3145.	2.5	54
5	When Are Tricoordinated Pd ^{II} Species Accessible? Stability Trends and Mechanistic Consequences. <i>Chemistry - A European Journal</i> , 2008, 14, 8986-8994.	1.7	50
6	Tailoring the gas separation efficiency of metal organic framework ZIF-8 through metal substitution: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4879-4892.	1.3	47
7	Catalysis and Mechanism of H ₂ Release from Amine-Boranes by Diron Complexes. <i>Inorganic Chemistry</i> , 2016, 55, 964-973.	1.9	34
8	On the Efficient Separation of Gas Mixtures with the Mixed-Linker Zeolitic-Imidazolate Framework-7-8. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 39631-39644.	4.0	32
9	Cyclopalladation and Reactivity of Amino Esters through C-H Bond Activation: Experimental, Kinetic, and Density Functional Theory Mechanistic Studies. <i>Chemistry - A European Journal</i> , 2013, 19, 17398-17412.	1.7	30
10	Proton-Transfer Reactions to Half-Sandwich Ruthenium Trihydride Complexes Bearing Hemilabile P,N Ligands: Experimental and Density Functional Theory Studies—Dedicated to Prof. Serafin Bernal in recognition of his contribution to inorganic chemistry, on the occasion of his retirement.. <i>Inorganic Chemistry</i> , 2010, 49, 6035-6057.	1.9	28
11	Computational Study of the Palladium-Catalyzed Carbonylative Synthesis of Aromatic Acid Chlorides: The Synergistic Effect of P <i>t</i> Bu ₃ and CO on Reductive Elimination. <i>Chemistry - A European Journal</i> , 2016, 22, 15107-15118.	1.7	27
12	Experimental and Computational Studies on the Iridium Activation of Aliphatic and Aromatic C-H Bonds of Alkyl Aryl Ethers and Related Molecules. <i>Chemistry - A European Journal</i> , 2009, 15, 9034-9045.	1.7	26
13	Molecular orbital analysis of the inverse halogen dependence of nuclear magnetic shielding in LaX ₃ , X = F, Cl, Br, I. <i>Magnetic Resonance in Chemistry</i> , 2010, 48, S76-S85.	1.1	26
14	Synthetic, Mechanistic, and Theoretical Studies on the Generation of Iridium Hydride Alkylidene and Iridium Hydride Alkene Isomers. <i>Chemistry - A European Journal</i> , 2009, 15, 9046-9057.	1.7	25
15	When Hartree-Fock exchange admixture lowers DFT-predicted barrier heights: Natural bond orbital analyses and implications for catalysis. <i>Journal of Chemical Physics</i> , 2018, 148, 244106.	1.2	25
16	Delayed Linker Addition (DLA) Synthesis for Hybrid SOD ZIFs with Unsubstituted Imidazolate Linkers for Propylene/Propane and n-Butane/i-Butane Separations. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 10103-10111.	7.2	23
17	Dehydrogenation of a tertiary amine-borane by a rhenium complex. <i>Chemical Communications</i> , 2014, 50, 5874-5877.	2.2	22
18	Defining New Limits in Gas Separations Using Modified ZIF Systems. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 20536-20547.	4.0	22

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19	Synthesis and catalytic activity of supported acenaphthoimidazolydene N-heterocyclic carbene ruthenium complex for ring closing metathesis (RCM) and ring opening metathesis polymerization (ROMP). <i>Journal of Catalysis</i> , 2016, 344, 100-107.	3.1	19
20	Green Light-Responsive CO-Releasing Polymeric Materials Derived from Ring-Opening Metathesis Polymerization. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 34376-34384.	4.0	19
21	Ancillary Ligand Effects upon the Photochemistry of Mn(bpy)(CO) ₃ X Complexes (X = Tj ETQq1 1 0.784314 rgBT /Overlo	1.9	16
22	A Benchmark Study of H ₂ Activation by Au ₃ and Ag ₃ Clusters. <i>Journal of Physical Chemistry C</i> , 2013, 117, 7487-7496.	1.5	15
23	Reactions of gold(III) complexes with alkenes in aqueous media: generation of bis-(<i>η</i> ² -hydroxyalkyl)gold(III) complexes. <i>Journal of Coordination Chemistry</i> , 2013, 66, 1153-1165.	0.8	15
24	Oxidative Addition of Haloalkanes to Metal Centers: A Mechanistic Investigation. <i>Organometallics</i> , 2014, 33, 3591-3595.	1.1	14
25	Computational investigation of the performance of ZIF-8 with encapsulated ionic liquids towards CO ₂ capture. <i>Molecular Physics</i> , 2019, 117, 3791-3805.	0.8	13
26	Mechanism of CO Displacement from an Unusually Labile Rhenium Complex: An Experimental and Theoretical Investigation. <i>Inorganic Chemistry</i> , 2012, 51, 13041-13049.	1.9	12
27	Thermal Dehydrogenation of Dimethylamine Borane Catalyzed by a Bifunctional Rhenium Complex. <i>Organometallics</i> , 2019, 38, 2602-2609.	1.1	12
28	Time Resolved Infrared Spectroscopy: Kinetic Studies of Weakly Binding Ligands in an Iron-iron Hydrogenase Model Compound. <i>Inorganic Chemistry</i> , 2012, 51, 7362-7369.	1.9	11
29	Why are GGAs so accurate for reaction kinetics on surfaces? Systematic comparison of hybrid vs. nonhybrid DFT for representative reactions. <i>Journal of Chemical Physics</i> , 2017, 146, 234103.	1.2	11
30	Data mining for predicting gas diffusivity in zeolitic-imidazolate frameworks (ZIFs). <i>Journal of Materials Chemistry A</i> , 2022, 10, 13697-13703.	5.2	11
31	The role of amide ligands in the stabilization of Pd(II) tricoordinated complexes: is the Pd-NR ₂ bond order single or higher?. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 75-84.	0.5	10
32	Ring opening metathesis polymerization (ROMP) and thio-bromo-click-chemistry approach toward the preparation of flame-retardant polymers. <i>Journal of Polymer Science Part A</i> , 2018, 56, 645-652.	2.5	10
33	Simulating Gold's Structure-Dependent Reactivity: Nonlocal Density Functional Theory Studies of Hydrogen Activation by Gold Clusters, Nanowires, and Surfaces. <i>Journal of Physical Chemistry C</i> , 2014, 118, 15693-15704.	1.5	9
34	Addition of ethylene to a π -conjugated two-dimensional nickel-based organometallic framework with implications for olefin separation. <i>Journal of Molecular Modeling</i> , 2015, 21, 107.	0.8	9
35	Nickel Bis(diselenolene) as a Catalyst for Olefin Purification. <i>Inorganic Chemistry</i> , 2016, 55, 10182-10191.	1.9	9
36	Estimating the strength of the M-H-B interaction: a kinetic approach. <i>Dalton Transactions</i> , 2013, 42, 6720.	1.6	8

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37	Carbon-hydrogen bond activation by a titanium neopentylidene complex. <i>Journal of Coordination Chemistry</i> , 2016, 69, 1759-1768.	0.8	8
38	Ligand Displacement Reaction Paths in a Diiron Hydrogenase Active Site Model Complex. <i>Chemistry - A European Journal</i> , 2016, 22, 12752-12760.	1.7	8
39	Transition-Metal-Free Homopolymerization of Pyrrolo[2,3- <i>d</i> :5,4- <i>d'</i>]-bisthiazoles via Nucleophilic Aromatic Substitution. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 41094-41101.	4.0	8
40	Methane Activations by Titanium Neopentylidene Complexes: Electronic Resilience and Steric Control. <i>Inorganic Chemistry</i> , 2017, 56, 9264-9272.	1.9	7
41	Mechanism of Ethylene Addition to Nickel Bis(oxathiolene) and Nickel Bis(dioxolene) Complexes. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7561-7568.	1.1	5
42	Delayed Linker Addition (DLA) Synthesis for Hybrid SOD ZIFs with Unsubstituted Imidazolate Linkers for Propylene/Propane and n-Butane/i-Butane Separations. <i>Angewandte Chemie</i> , 2021, 133, 10191-10199.	1.6	5
43	Light-Enhanced Displacement of Methyl Acrylate from Iron Carbonyl: Investigation of the Reactive Intermediate via Rapid-Scan Fourier Transform Infrared and Computational Studies. <i>Inorganic Chemistry</i> , 2013, 52, 12655-12660.	1.9	3
44	Simulating periodic trends in the structure and catalytic activity of coinage metal nanoribbons. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1718-1725.	1.0	3
45	Reversible Olefin Addition to Extended Lattices of a Nickel-Selenium Framework. <i>Journal of Physical Chemistry C</i> , 2018, 122, 22424-22434.	1.5	2
46	One-Pot Tandem Ring-Opening and Ring-Closing Metathesis Polymerization of Disubstituted Cyclopentenes Featuring a Terminal Alkyne Functionality. <i>Macromolecules</i> , 2020, 53, 4330-4337.	2.2	1
47	The Chemistry of Short-Lived $\hat{\pm}$ -Fluorocarocations. <i>Journal of Organic Chemistry</i> , 2021, 86, 3882-3889.	1.7	1
48	Detection of an unusual intermediate in the photolysis of an iron tricarbonyl complex. <i>Journal of Organometallic Chemistry</i> , 2017, 851, 189-193.	0.8	0
49	What Happens Without Nickel? Cyclization Reactions of Ethylene with Ethanedithial and Related Molecules. <i>Journal of Computational Chemistry</i> , 2018, 39, 1158-1167.	1.5	0
50	Tunable model promoters in DFT simulations of catalysts. <i>Journal of Computational Chemistry</i> , 2019, 40, 1752-1757.	1.5	0
51	Computational investigation of cobalt and copper bis(oxathiolene) complexes as an alternative for olefin purification. <i>Journal of Molecular Modeling</i> , 2020, 26, 205.	0.8	0