

Carlo Alberto Gaggioli

List of Publications by Year in descending order

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papers

908
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430442

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times ranked

1583
citing authors

#	ARTICLE	IF	CITATIONS
1	Tuning the Properties of Zr ₆ O ₈ Nodes in the Metal Organic Framework UiO-66 by Selection of Node-Bound Ligands and Linkers. <i>Chemistry of Materials</i> , 2019, 31, 1655-1663.	3.2	97
2	Tuning Catalytic Sites on Zr ₆ O ₈ Metal-Organic Framework Nodes via Ligand and Defect Chemistry Probed with <i>tert</i> -Butyl Alcohol Dehydration to Isobutylene. <i>Journal of the American Chemical Society</i> , 2020, 142, 8044-8056.	6.6	83
3	Globularity-Selected Large Molecules for a New Generation of Multication Perovskites. <i>Advanced Materials</i> , 2017, 29, 1702005.	11.1	81
4	Beyond Density Functional Theory: The Multiconfigurational Approach To Model Heterogeneous Catalysis. <i>ACS Catalysis</i> , 2019, 9, 8481-8502.	5.5	75
5	Effects of Covalency on Anionic Redox Chemistry in Semiquinoid-Based Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2020, 142, 2653-2664.	6.6	75
6	A Tunable Multivariate Metal-Organic Framework as a Platform for Designing Photocatalysts. <i>Journal of the American Chemical Society</i> , 2021, 143, 6333-6338.	6.6	69
7	Modulating the Bonding Properties of <i>N</i> -Heterocyclic Carbenes (NHCs): A Systematic Charge-Displacement Analysis. <i>Chemistry - A European Journal</i> , 2017, 23, 7558-7569.	1.7	45
8	Strong Electron-Donating Ligands Accelerate the Protodeauration Step in Gold(I)-Catalyzed Reactions: A Quantitative Understanding of the Ligand Effect. <i>Organometallics</i> , 2016, 35, 2275-2285.	1.1	41
9	Synthesis and Characterization of Tris-chelate Complexes for Understanding <i>f</i> -Orbital Bonding in Later Actinides. <i>Journal of the American Chemical Society</i> , 2019, 141, 2356-2366.	6.6	41
10	C-H Bond Activation on Bimetallic Two-Atom Co-M Oxide Clusters Deposited on Zr-Based MOF Nodes: Effects of Doping at the Molecular Level. <i>ACS Catalysis</i> , 2018, 8, 2864-2869.	5.5	39
11	Dioxygen insertion into the gold(<i>h</i>)-hydride bond: spin orbit coupling effects in the spotlight for oxidative addition. <i>Chemical Science</i> , 2016, 7, 7034-7039.	3.7	33
12	Theoretical Investigation of Plutonium-Based Single-Molecule Magnets. <i>Inorganic Chemistry</i> , 2018, 57, 8098-8105.	1.9	29
13	Hydrogen Atom or Proton Coupled Electron Transfer? C-H Bond Activation by Transition-Metal Oxides. <i>Journal of the American Chemical Society</i> , 2019, 141, 14603-14611.	6.6	25
14	Spin-Forbidden Reactions: Adiabatic Transition States Using Spin-Orbit Coupled Density Functional Theory. <i>Chemistry - A European Journal</i> , 2018, 24, 5006-5015.	1.7	23
15	Synthesis and characterization of tetrairidium clusters in the metal organic framework UiO-67: Catalyst for ethylene hydrogenation. <i>Journal of Catalysis</i> , 2020, 382, 165-172.	3.1	23
16	Cu[Ni(2,3-pyrazinedithiolate) ₂] Metal-Organic Framework for Electrocatalytic Hydrogen Evolution. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 34419-34427.	4.0	23
17	Bioinspired Nickel Complexes Supported by an Iron Metalloligand. <i>Inorganic Chemistry</i> , 2020, 59, 14251-14262.	1.9	20
18	The ligand effect on the oxidative addition of dioxygen to gold(<i>h</i>)-hydride complexes. <i>Dalton Transactions</i> , 2017, 46, 11679-11690.	1.6	19

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19	Using Redox-Active Ligands to Generate Actinide Ligand Radical Species. <i>Inorganic Chemistry</i> , 2021, 60, 15242-15252.	1.9	19
20	Cyclization of 2-Alkynyldimethylaniline on Gold(I) Cationic and Neutral Complexes. <i>Organometallics</i> , 2016, 35, 595-604.	1.1	18
21	Active Learning Configuration Interaction for Excited-State Calculations of Polycyclic Aromatic Hydrocarbons. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7518-7530.	2.3	12
22	DFT Study on the Catalytic Activity of ALD-Grown Diiron Oxide Nanoclusters for Partial Oxidation of Methane to Methanol. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1580-1592.	1.1	7
23	Evidence of Alpha Radiolysis in the Formation of a Californium Nitrate Complex. <i>Chemistry - A European Journal</i> , 2020, 26, 8885-8888.	1.7	6
24	Singlet-to-Triplet Spin Transitions Facilitate Selective 1-Butene Formation during Ethylene Dimerization in Ni(II)-MFU-4 <i>l</i> . <i>Journal of Physical Chemistry C</i> , 2021, 125, 22036-22043.	1.5	5
25	Frontispiece: Spin-Forbidden Reactions: Adiabatic Transition States Using Spin-Orbit Coupled Density Functional Theory. <i>Chemistry - A European Journal</i> , 2018, 24, .	1.7	0