

Varinia S Bernales

List of Publications by Year in descending order

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31
papers

2,295
citations

236925

25
h-index

454955

30
g-index

31
all docs

31
docs citations

31
times ranked

3360
citing authors

#	ARTICLE	IF	CITATIONS
1	Sintering-Resistant Single-Site Nickel Catalyst Supported by Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2016, 138, 1977-1982.	13.7	273
2	Quantum Mechanical Continuum Solvation Models for Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9122-9129.	2.6	225
3	Metal-Organic Framework Supported Cobalt Catalysts for the Oxidative Dehydrogenation of Propane at Low Temperature. <i>ACS Central Science</i> , 2017, 3, 31-38.	11.3	222
4	Catalytic Silylation of Dinitrogen with a Dicobalt Complex. <i>Journal of the American Chemical Society</i> , 2015, 137, 4638-4641.	13.7	162
5	Tuning the Surface Chemistry of Metal Organic Framework Nodes: Proton Topology of the Metal-Oxide-Like Zr ₆ Nodes of UiO-66 and NU-1000. <i>Journal of the American Chemical Society</i> , 2016, 138, 15189-15196.	13.7	155
6	Structure and Dynamics of Zr ₆ O ₈ Metal-Organic Framework Node Surfaces Probed with Ethanol Dehydration as a Catalytic Test Reaction. <i>Journal of the American Chemical Society</i> , 2018, 140, 3751-3759.	13.7	150
7	Computational Design of Functionalized Metal-Organic Framework Nodes for Catalysis. <i>ACS Central Science</i> , 2018, 4, 5-19.	11.3	148
8	Computationally Guided Discovery of a Catalytic Cobalt-Decorated Metal-Organic Framework for Ethylene Dimerization. <i>Journal of Physical Chemistry C</i> , 2016, 120, 23576-23583.	3.1	78
9	Bimetallic Cobalt-Dinitrogen Complexes: Impact of the Supporting Metal on N ₂ Activation. <i>Inorganic Chemistry</i> , 2015, 54, 9263-9270.	4.0	77
10	Bridging Zirconia Nodes within a Metal-Organic Framework via Catalytic Ni-Hydroxo Clusters to Form Heterobimetallic Nanowires. <i>Journal of the American Chemical Society</i> , 2017, 139, 10410-10418.	13.7	74
11	Molecular Rhodium Complexes Supported on the Metal-Oxide-Like Nodes of Metal Organic Frameworks and on Zeolite HY: Catalysts for Ethylene Hydrogenation and Dimerization. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 33511-33520.	8.0	69
12	Density matrix renormalization group pair-density functional theory (DMRG-PDFT): singlet-triplet gaps in polyacenes and polyacetylenes. <i>Chemical Science</i> , 2019, 10, 1716-1723.	7.4	69
13	Installing Heterobimetallic Cobalt-Aluminum Single Sites on a Metal Organic Framework Support. <i>Chemistry of Materials</i> , 2016, 28, 6753-6762.	6.7	56
14	Unprecedented selectivity in molecular recognition of carbohydrates by a metal-organic framework. <i>Chemical Communications</i> , 2016, 52, 7094-7097.	4.1	49
15	Structural and Spectroscopic Characterization of Reaction Intermediates Involved in a Dinuclear Co-H ₂ O ₂ Water Oxidation Catalyst. <i>Journal of the American Chemical Society</i> , 2016, 138, 15291-15294.	13.7	49
16	Heterobimetallic Complexes That Bond Vanadium to Iron, Cobalt, and Nickel. <i>Inorganic Chemistry</i> , 2015, 54, 11669-11679.	4.0	45
17	Atomic Layer Deposition in a Metal-Organic Framework: Synthesis, Characterization, and Performance of a Solid Acid. <i>Chemistry of Materials</i> , 2017, 29, 1058-1068.	6.7	45
18	Computational Study of First-Row Transition Metals Supported on MOF NU-1000 for Catalytic Acceptorless Alcohol Dehydrogenation. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24697-24705.	3.1	40

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19	Câ€“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.	11.2	39
20	Can Density Matrix Embedding Theory with the Complete Activate Space Self-Consistent Field Solver Describe Single and Double Bond Breaking in Molecular Systems?. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1960-1968.	5.3	39
21	Effect of Unsaturation on the Absorption of Ethane and Ethylene in Imidazolium-Based Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2013, 117, 7416-7425.	2.6	36
22	Negative cooperativity upon hydrogen bond-stabilized O2 adsorption in a redox-active metalâ€“organic framework. <i>Nature Communications</i> , 2020, 11, 3087.	12.8	36
23	Computationally-Guided Assignment of Unexpected Signals in the Raman Spectra of Uranyl Triperoxide Complexes. <i>Inorganic Chemistry</i> , 2017, 56, 1574-1580.	4.0	35
24	Enhanced Fe-Centered Redox Flexibility in Feâ€“Ti Heterobimetallic Complexes. <i>Inorganic Chemistry</i> , 2019, 58, 6199-6214.	4.0	29
25	Valence ï€“ Excitations in Benzene Studied by Multiconfiguration Pair-Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 75-81.	4.6	29
26	Uranyl Peroxide Cage Cluster Solubility in Water and the Role of the Electrical Double Layer. <i>Inorganic Chemistry</i> , 2017, 56, 1333-1339.	4.0	27
27	Catalytic descriptors and electronic properties of single-site catalysts for ethene dimerization to 1-butene. <i>Catalysis Today</i> , 2018, 312, 149-157.	4.4	16
28	Rhodium catalyzed hydroformylation of olefins. <i>Journal of Computational Chemistry</i> , 2019, 40, 342-348.	3.3	12
29	Isobutane as a probe of the structure of 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquids. <i>Journal of Chemical Thermodynamics</i> , 2015, 89, 98-103.	2.0	9
30	Correction to â€œComputationally Guided Discovery of Catalytic Cobalt-Decorated Metalâ€“Organic Framework for Ethylene Dimerizationâ€“. <i>Journal of Physical Chemistry C</i> , 2017, 121, 11975-11975.	3.1	2
31	The role of cations in uranyl nanocluster association: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 1847-1854.	2.8	0