# Varinia S Bernales

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6437516/publications.pdf

Version: 2024-02-01

| | | | |
|---|---|---|---|
| 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 | The role of cations in uranyl nanocluster association: a molecular dynamics study. Physical Chemistry Chemical Physics, 2020, 22, 1847-1854. | 2.8 | 0 |
| 2 | Negative cooperativity upon hydrogen bond-stabilized O2 adsorption in a redox-active metalâ€“organic framework. Nature Communications, 2020, 11, 3087. | 12.8 | 36 |
| 3 | Enhanced Fe-Centered Redox Flexibility in Feâ€“Ti Heterobimetallic Complexes. Inorganic Chemistry, 2019, 58, 6199-6214. | 4.0 | 29 |
| 4 | Density matrix renormalization group pair-density functional theory (DMRG-PDFT): singletâ€“triplet gaps in polyacenes and polyacetylenes. Chemical Science, 2019, 10, 1716-1723. | 7.4 | 69 |
| 5 | Rhodium catalyzed hydroformylation of olefins. Journal of Computational Chemistry, 2019, 40, 342-348. | 3.3 | 12 |
| 6 | Valence ï€ï€* Excitations in Benzene Studied by Multiconfiguration Pair-Density Functional Theory. Journal of Physical Chemistry Letters, 2019, 10, 75-81. | 4.6 | 29 |
| 7 | Catalytic descriptors and electronic properties of single-site catalysts for ethene dimerization to 1-butene. Catalysis Today, 2018, 312, 149-157. | 4.4 | 16 |
| 8 | 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. ACS Catalysis, 2018, 8, 2864-2869. | 11.2 | 39 |
| 9 | Structure and Dynamics of Zr<sub>6</sub>O<sub>8</sub> Metalâ€“Organic Framework Node Surfaces Probed with Ethanol Dehydration as a Catalytic Test Reaction. Journal of the American Chemical Society, 2018, 140, 3751-3759. | 13.7 | 150 |
| 10 | Computational Design of Functionalized Metalâ€“Organic Framework Nodes for Catalysis. ACS Central Science, 2018, 4, 5-19. | 11.3 | 148 |
| 11 | Can Density Matrix Embedding Theory with the Complete Activate Space Self-Consistent Field Solver Describe Single and Double Bond Breaking in Molecular Systems?. Journal of Chemical Theory and Computation, 2018, 14, 1960-1968. | 5.3 | 39 |
| 12 | Atomic Layer Deposition in a Metalâ€“Organic Framework: Synthesis, Characterization, and Performance of a Solid Acid. Chemistry of Materials, 2017, 29, 1058-1068. | 6.7 | 45 |
| 13 | Computationally-Guided Assignment of Unexpected Signals in the Raman Spectra of Uranyl Triperoxide Complexes. Inorganic Chemistry, 2017, 56, 1574-1580. | 4.0 | 35 |
| 14 | Uranyl Peroxide Cage Cluster Solubility in Water and the Role of the Electrical Double Layer. Inorganic Chemistry, 2017, 56, 1333-1339. | 4.0 | 27 |
| 15 | Correction to â€œComputationally Guided Discovery of Catalytic Cobalt-Decorated Metalâ€“Organic Framework for Ethylene Dimerizationâ€• Journal of Physical Chemistry C, 2017, 121, 11975-11975. | 3.1 | 2 |
| 16 | Metalâ€“Organic Framework Supported Cobalt Catalysts for the Oxidative Dehydrogenation of Propane at Low Temperature. ACS Central Science, 2017, 3, 31-38. | 11.3 | 222 |
| 17 | Molecular Rhodium Complexes Supported on the Metal-Oxide-Like Nodes of Metal Organic Frameworks and on Zeolite HY: Catalysts for Ethylene Hydrogenation and Dimerization. ACS Applied Materials & Interfaces, 2017, 9, 33511-33520. | 8.0 | 69 |
| 18 | Bridging Zirconia Nodes within a Metalâ€“Organic Framework via Catalytic Ni-Hydroxo Clusters to Form Heterobimetallic Nanowires. Journal of the American Chemical Society, 2017, 139, 10410-10418. | 13.7 | 74 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Unprecedented selectivity in molecular recognition of carbohydrates by a metalâ€“organic framework. Chemical Communications, 2016, 52, 7094-7097. | 4.1 | 49 |
| 20 | Installing Heterobimetallic Cobaltâ€“Aluminum Single Sites on a Metal Organic Framework Support. Chemistry of Materials, 2016, 28, 6753-6762. | 6.7 | 56 |
| 21 | Computationally Guided Discovery of a Catalytic Cobalt-Decorated Metalâ€“Organic Framework for Ethylene Dimerization. Journal of Physical Chemistry C, 2016, 120, 23576-23583. | 3.1 | 78 |
| 22 | Computational Study of First-Row Transition Metals Supported on MOF NU-1000 for Catalytic Acceptorless Alcohol Dehydrogenation. Journal of Physical Chemistry C, 2016, 120, 24697-24705. | 3.1 | 40 |
| 23 | Tuning the Surface Chemistry of Metal Organic Framework Nodes: Proton Topology of the Metal-Oxide-Like Zr<sub>6</sub> Nodes of UiO-66 and NU-1000. Journal of the American Chemical Society, 2016, 138, 15189-15196. | 13.7 | 155 |
| 24 | Structural and Spectroscopic Characterization of Reaction Intermediates Involved in a Dinuclear Coâ€“Hbpp Water Oxidation Catalyst. Journal of the American Chemical Society, 2016, 138, 15291-15294. | 13.7 | 49 |
| 25 | Sintering-Resistant Single-Site Nickel Catalyst Supported by Metalâ€“Organic Framework. Journal of the American Chemical Society, 2016, 138, 1977-1982. | 13.7 | 273 |
| 26 | Isobutane as a probe of the structure of 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquids. Journal of Chemical Thermodynamics, 2015, 89, 98-103. | 2.0 | 9 |
| 27 | Heterobimetallic Complexes That Bond Vanadium to Iron, Cobalt, and Nickel. Inorganic Chemistry, 2015, 54, 11669-11679. | 4.0 | 45 |
| 28 | Bimetallic Cobaltâ€“Dinitrogen Complexes: Impact of the Supporting Metal on N<sub>2</sub> Activation. Inorganic Chemistry, 2015, 54, 9263-9270. | 4.0 | 77 |
| 29 | Catalytic Silylation of Dinitrogen with a Dicobalt Complex. Journal of the American Chemical Society, 2015, 137, 4638-4641. | 13.7 | 162 |
| 30 | Effect of Unsaturation on the Absorption of Ethane and Ethylene in Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2013, 117, 7416-7425. | 2.6 | 36 |
| 31 | Quantum Mechanical Continuum Solvation Models for Ionic Liquids. Journal of Physical Chemistry B, 2012, 116, 9122-9129. | 2.6 | 225 |