Computationally Guided Discovery of Metal-Decorated Metal–Organic Frameworks Active for Catalysis
Laura Gagliardi

Department of Chemistry, Chemical Theory Center, and Supercomputing Institute, University of Minnesota, Minneapolis, Minnesota 55455-0431, United States

Metal-organic frameworks (MOFs) are attracting the attention of many scientists because of their high selectivity in gas separations, catalytic activity, and magnetic properties. We have combined theory and experiment to understand the activity of nickel, cobalt, and rhodium catalysts supported on Zr₆ nodes in metal–organic frameworks (MOFs) for reactions related to natural gas manipulation. For Ni and Co,¹ ² computational studies provide important insights with respect to the catalytic mechanism(s) for observed ethylene dimerization after metal-decoration of the MOF NU-1000. Rh complexes have been installed on the Zr₆ nodes of not only NU-1000, but also the related metal–organic framework UiO-67, and the zeolite DAY; influences of the supports on ethylene hydrogenation and dimerization have been assessed. A library of transition metals (TMs), ranging from first row TMs to noble metals, is now being screened computationally to search for optimal catalysts, and structure-function relationships are beginning to emerge from this theory-driven approach.


The structure of the NU1000 metal-organic framework.