Center for the Computational Design of Functional Layered Materials

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

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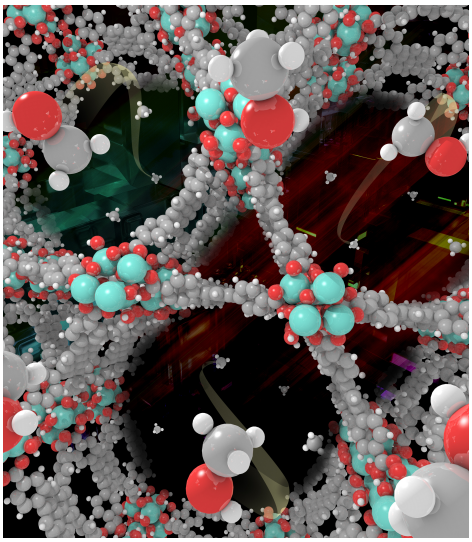

Metal-organic frameworks (MOFs) are attracting the attention of many scientists because of their high selectivity in gas separations, catalytic activity, and magnetic properties. We have combined theory and experiment to understand the activity of nickel, cobalt, and rhodium catalysts supported on Zr_6 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. 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.[3]

1. V. Bernales, A. B. League, Z. Li, N. M. Schweitzer, A. W. Peters, R. K. Carlson, J. T. Hupp, C. J. Cramer, O. K. Farha, and L. Gagliardi, *Computationally-Guided Discovery of Catalytic Cobalt-Decorated Metal–Organic Framework for Ethylene Dimerization*, J. Phys. Chem. C., 120, 23576–23583 (2016)
2. J. Ye, L. Gagliardi, C. J. Cramer, D. G. Truhlar, *Single Ni atoms and Ni_4 clusters have similar catalytic activity for ethylene dimerization* J. of Catalysis, 354, 278-286 (2017
3. M. C. Simons, M. A. Ortuño, V. Bernales, C. J. Cramer, A. Bhan, and L. Gagliardi, *C–H Bond activation on bimetallic two-atom Co-M oxide clus-ters deposited on Zr-based MOF nodes: Effects of doping at the molecular level* Submitted (2017)

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Laura Gagliardi's interest is focused on the development of novel quantum chemical methods for strongly correlated systems She combines first-principle methods with classical simulation techniques. The applications are focused on the computational design of novel materials and molecular systems for energy-related challenges. Special focus is devoted to modeling catalysis and spectroscopy in molecular systems; catalysis and gas separation in porous materials; photovoltaic properties of organic and inorganic semiconductors; separation of actinides. She published more than 270 peer-reviewed papers.