UCMERCED
UNIVERSITY OF CALIFORNIA
School of Natural Sciences

CHEMISTRY SEMINAR 291

Computational Design of Functionalized Metal–Organic Framework for Catalysis

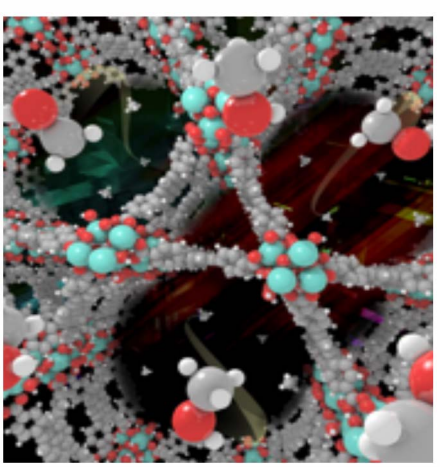
Laura Gagliardi
Department of Chemistry, Chemical Theory Center, and Supercomputing Institute
University of Minnesota

Date:**10/26/18**
Time: **3:00 PM**
Location: **COB1 267**

For more information contact:
Hrant Hratchian
hhratchian@ucmerced.edu

ABSTRACT

We employ computational modeling1 to understand the activity of metal catalysts supported on Zr6 nodes in metal–organic frameworks (MOFs) for reactions related to natural gas conversion, like catalytic oligomerization of abundant C1, C2, and C3 hydrocarbons to longer congeners or selective oxidation to alcohols or other fuel molecules, while avoiding overoxidation to water and carbon dioxide. For Ni and Co,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, M. A. Ortuño, D. G. Truhlar, C. J. Cramer, and L. Gagliardi, Computational Design of Functionalized Metal–Organic Framework Nodes for Catalysis, ACS Cent. Sci., 4, 5-19 (2018)

2 J. Ye, L. Gagliardi, C. J. Cramer, D. G. Truhlar, Single Ni atoms and Ni4 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 ACS Cat. 8, 2864–2869 (2018)