Computational characterization of catalytic processes: homogenous and heterogeneous

Laura Gagliardi

Department of Chemistry, Supercomputing Institute, and Chemical Theory Center,
University of Minnesota, Minneapolis, Minnesota, 55455, USA
gagliard@umn.edu

Computational chemistry is a fundamental tool for the understanding and prediction of catalytic processes. I will discuss the challenges of quantum chemical studies on homo- and heterobimetallic compounds featuring metal-metal multiple bonds[1] and their utilization for various catalytic reactions, including the silylation of dinitrogen.[2] In the second part of my talk, I will describe our recent efforts on the post-synthetic functionalization of Zr_6-based metal-organic frameworks to imbue them with catalytic properties.[3]

[1] R. K. Carlson, S. O. Odoh, S. J. Tereniak, C. C. Lu, and L. Gagliardi, *Can Multiconfigurational Self-Consistent Field Theory and Density Functional Theory Correctly Predict the Ground State of Metal–Metal-Bonded Complexes*? J. Chem. Theory Comput. **11**, 2015, pp 4093–4101.

[2] R. B. Siedschlag, V. Bernales, K. D. Vogiatzis, N. Planas, L. J. Clouston, E. Bill, L. Gagliardi, and C. C. Lu, *Catalytic Silylation of Dinitrogen with a Dicobalt Complex*, J. Am. Chem. Soc., **137,** 2015, pp 4638-4641.

[3] D. Yang, S. O. Odoh, T. C. Wang, O. K. Farha, J. T. Hupp, C. J. Cramer, L. Gagliardi, and B. C. Gates, *Metal-Organic Framework Nodes as Nearly Ideal Supports for Molecular Catalysts: NU-1000 and UiO-66-Supported Iridium Complexes*, J. Am. Chem. Soc., **137**, 2015, pp 7391–7396.

Calculated mechanism for the dicobalt-mediated silylation of N_2