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# NCCR MARVEL Distinguished Lecture

# Homogenous and heterogeneous catalysis: two challenges for modern quantum chemistry

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**Abstract:** Quantum chemistry is a fundamental tool for the understanding and prediction of catalytic processes. I will discuss our computational studies on homo- and heterobimetallic compounds featuring metal-metal multiple bonds and their reactivity.[1] Various quantum chemical methods are employed to study these systems, ranging from Kohn-Sham density functional theory to our newly developed multireference version of density functional theory.[2] I will then discuss our recent investigations of supported Ni and Co catalysts at the $Zr_6$ node of the metal-organic framework NU-1000. These systems exhibit interesting properties in catalyzing ethylene dimerization and hydrogenation. Computational studies reveal important insights regarding the possible mechanisms of the catalysis.[3] A library of transition metals is now under investigation, in order to screen for the best catalyst, and structure-function relationships are beginning to emerge from computational screening.

**References:**

[1] 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.*, 2015, 137, 4638-4641.

[2] S. O. Odoh, G. L. Manni, R. K. Carlson, C. G. Truhlar, and L. Gagliardi, "Separated-pair approximation and separated-pair pair-density functional theory", *Chem. Sci.,* 2016, 7, 2399-2413.

[3] Z. Li, N. M. Schweitzer, A. B. League, V. Bernales, A. W. Peters, A. B. Getsoian, T. C. Wang, J. T. Miller, A. Vjunov, J. L. Fulton, J. A. Lercher, C. J. Cramer, L. Gagliardi, J. T. Hupp, O. K. Farha, "Sintering-Resistant Single-Site Nickel Catalyst Supported by Metal-Organic Framework", *J. Am. Chem. Soc.,* 2016, 138, 1977-1982.