"ADVENTURES IN CATALYSIS: COMPUTATION AND EXPERIMENT"

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Detailed understanding of catalytic transformations is key to designing better catalysts. This talk will give insights on case studies and reactivity designs recently undertaken in our laboratory. A combination of experimental and computational tools were applied to study and/or predict the favored reaction mechanisms, active catalytic species, ligand and additive effects of selected transformations relating to C-C bond formations, C-H functionalizations and the introduction of fluorine containing groups, catalyzed by palladium, nickel and/or Cu complexes of the oxidation states 0, I, II or III. As a result of these investigations, novel reactivities have been uncovered. The lecture will also discuss the power and limitations of computational tools in the study of organic and organometallic reactivities, and outline the advantages of a combined experimental/ computational approach.[1]

References:
1) a) Sperger, T.; Sanhueza, I. A.; Kalvet, I.; Schoenebeck, F. *Chem. Rev.* **2015**, *115*, 9532. b) Bonney, K. J.; Schoenebeck, F. *Chem. Soc. Rev.* **2014**, *43*, 6609; c) Tsang, A. S.-K.; Sanhueza, I. A.; Schoenebeck, F. *Chem. Eur. J.* **2014**, *20*, 16432.