Ph.D. Open Seminar

Department of Chemistry

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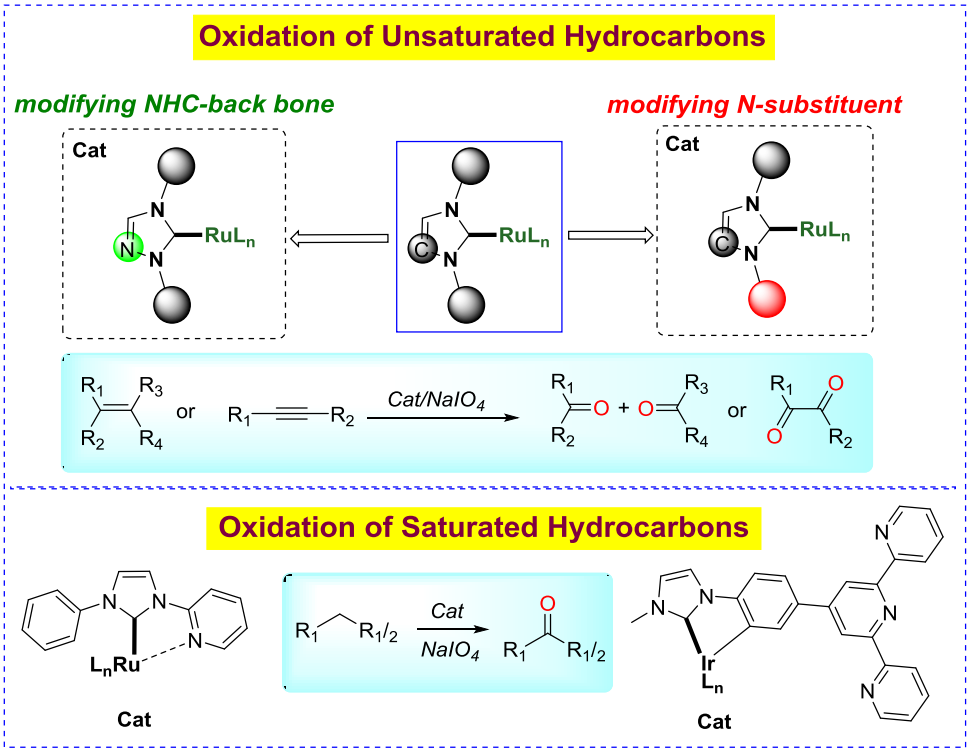
Topic of Seminar: Exploring Electronically Modulated Discrete Ruthenium(II) and Iridium(III)-NHC Complexes as Hydrocarbon Oxidation Pre-catalysts

Date: December 21, 2016 **Time:** 4.00 PM **Venue:** AB-II (401)

Abstract:

Oxyfunctionalization of hydrocarbons, catalyzed by metal complexes, to valuable organic derivatives is a challenging research area in organometallic chemistry.[1] Ligand backbone in such metal complexes undoubtedly plays a vital role in controlling the stereoelectronic properties of the catalysts which, in turn, influence the catalytic outcome in terms of selectivity and reactivity. Therefore, efforts are made to tune the electronic properties of man-made catalysts for better understanding and/or performance of the same. Due to the robustness provided by the NHCs to the catalyst under the harsh reaction conditions and ease of tuning their stereoelectronic properties, NHCs have placed themselves in the front row of the ligand matrix as developed and utilized successfully in various fields of fundamental organometallic chemistry.[2] My thesis work has been conceived with the above background to address the rational design of efficient metal-NHC pre-catalysts in the context of oxyfunctionalization of saturated and unsaturated hydrocarbon molecules. In this seminar, how the electronic properties of ruthenium(II) and iridium(III) metal centers can be tuned within NHC-backbone will be discussed.[3] Furthermore, the application of these NHC-based ruthenium(II) and iridium(III) complexes towards the oxidative functionalization of hydrocarbons, sp^3 C-H bonds[3b,4] and carbon-carbon multiple bonds[5], will be presented. More importantly, the alteration of catalytic turnovers resulted by the electronic tuning within the NHC-backbone for the highly selective catalytic cleavage of carbon-carbon multiple bonds will also be explained.[5]



References:

[1] Zhou, M.; Crabtree, R. H. *Chem. Soc. Rev.* **2011**, *40*, 1875. [2] Hopkinson, M. N.; Richter, C.; Schedler, M.; Glorius, F. *Nature* **2014**, *510*, 485. [3] (a) Mondal, M.; Thenarukandiyil, R.; Gupta, S. K.; Choudhury, J. *Dalton Trans.* **2014**, *43*, 9356; (b) Gupta, S. K.; Choudhury, J. *Dalton Trans*. **2015**, *44*, 1233. [4] Gupta, S. K.; Choudhury, J. *Manuscript submitted*. [5] (a) Gupta, S. K.; Choudhury, J. *Chem. Commun.* **2016**, *52*, 3384; (b) Gupta, S. K.; Sahoo, S. K.; Choudhury, J. *Organometallics* **2016**, *35*, 2462; (c) Gupta, S. K.; Choudhury, J. *Manuscript under preparation.*