

# PhD Open Seminar

Department of Chemistry, IISER Bhopal

Title of the Thesis: *Annulative  $\pi$ -Extension (APEX) with Metal–N-Heterocyclic Carbene Templates: A Unique Strategy toward New Classes of Cationic Polycyclic Heteroarenes*

Speaker: Champak Dutta  
Date: 17.05.2019

Thesis Supervisor: Dr. Joyanta Choudhury  
Venue: AB-II 401

Roll No: 1410202  
Time: 11:00 AM

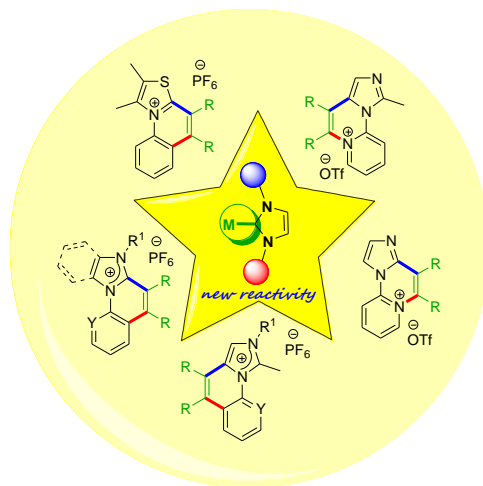
## Abstract

Beyond the well-known unique ligand property of metal-templated NHCs (NHC = N-heterocyclic carbene),<sup>[1]</sup> a new facet of these species has been revealed recently and found to be of significant interest in catalysis and materials research.<sup>[2]</sup> This new aspect features an unprecedented chemistry of Rh–NHC backbone which was made active in *catalytic intermolecular annulation* of imidazolium motifs with internal alkynes leading to the synthesis of a variety of highly conjugated, cationic and annulated organic molecules.<sup>[2,3]</sup>

Based on the above background, the primary aim of the present thesis work was to address the quest of (a) new class of ‘*azolium*’ substrates suitable for above strategy, (b) new annulation pattern suitable for variable optoelectronic property of the products, and (c) new catalyst system conducive for such type of challenging annulation reactions.

The first question was successfully addressed *via* demonstrating the Rh-catalyzed annulation strategy on N,S-heterocyclic carbene (NSHC) motifs accessed from thiazolium compounds, thus forming a new class of doubly doped thiazoloquinolinium scaffolds with tunable fluorescence and electronic properties.<sup>[4]</sup> Next, an interesting bimodal ‘*rollover annulation*’ pattern was developed using 2-heteroarylimidazolium motifs with the Rh(III) catalyst system showing annulation *via* reductive elimination and alkenylation *via* protodemetalation process.<sup>[5,6]</sup> Finally, a new alternative catalyst system based on Co(III) replacing Rh(III) was discovered, which was found to catalyze an interesting C–N annulation *via* the involvement of unprecedented ‘*protic-NHC–Co*’ templates.<sup>[7]</sup>

In this seminar, all the above results will be discussed in detail.



## *References:*

- [1] Hopkinson, M. N.; Richter, C.; Schedler, M.; Glorius, F. *Nature* **2014**, *510*, 485-496.
- [2] Ghorai, D.; Choudhury, J. *Chem. Commun.* **2014**, *50*, 15159-15162.
- [3] (a) Ghorai, D.; Choudhury, J. *ACS Catal.* **2015**, *5*, 2692-2696; (b) Thenarukandiyil, R.; Gupta, S. K.; Choudhury, J. *ACS Catal.* **2016**, *6*, 5132-5137; (c) Thenarukandiyil, R.; Dutta, C.; Choudhury, J. *Chem. - Eur. J.* **2017**, *23*, 15529-15533; (d) Dutta, C.; Choudhury, J. *RSC Adv.* **2018**, *8*, 27881-27891 (review).
- [4] Dutta, C.; Sainaba, A. B.; Choudhury, J. *Chem. Commun.* **2019**, *55*, 854-857.
- [5] Ghorai, D.; Dutta, C.; Choudhury, J. *ACS Catal.* **2016**, *6*, 709-713.
- [6] Dutta, C.; Ghorai, D.; Choudhury, J. *ACS Omega* **2018**, *3*, 1614-1620.
- [7] Dutta, C.; Choudhury, J. *Manuscript under preparation.*