2E20

Computational Insight into the C-H functionalization Jungle

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I will present our collaborative approaches to the transition metal catalyzed C-H bond functionalization. At first, I will elaborate our efforts on understanding the di-Rh, di-Ru, (pybox)Ru catalyzed C-H bond alkylation and amination reactions. I will analyze the factors controlling the reactivity of these complexes and make intriguing predictions. I will apply of those principles to predict the (PDI)Fe-catalyst for the C-H bond alkylation. In the second part of my presentation, I will demonstrate results from our recently discovered mono-protected amino acid ligands (MPAA) promoted Pd(II)-catalyzed enantioselective C–H activation reaction with both pyridine and carboxylic acid directing groups. Presented computational investigations allowed us to gain insights into the mechanisms and important elementary steps of the reaction, nature of active species, a ligand coordination mode to the Pd(II), transition state structure of the C–H activation step and base effect.