

Characterization and physicochemical properties of Ir(I) complexes on bipyridine-based covalent triazine framework

ABSTRACT

Ir-complexes containing bipyridine-based ligands have shown superior performance in heterogeneous catalysis with superior activity and selectivity [1]. Bipyridine-based covalent triazine framework (bipy-CTF) have been functionalized via post-metalation with a dimer complex $[\text{Ir}(\text{OMe})(\text{cod})]_2$ for borylation reactions [2]. Physical characterization of the immobilized Ir(I) complex onto bipy-CTF in combination with the computational calculations showed a high stabilization energy of the Ir(I) complex moiety in the frameworks with the presence of boron reagent, bis(pinacolato)diboron. The comparison values of calculated and experimental BET surface area and pore volume indicates that most of the complexes are inside the pores of bipy-CTF framework. For the surface prepared with Ir, X-ray absorption spectroscopy at the Ir-L3 edge showed an edge energy as well as post-edge features that were essentially identical with those observed theoretically [3]. Density functional theory (DFT) calculations demonstrates that the Ir(I) complex was anchored to the framework through the two N atoms of bipy and were actual active for the borylation reaction in the presence of bis(pinacolato)diboron (Fig. 1) [4].