Heme metal-oxygen utilizing catalysts (M=O, M-OO, M-OOH, M-HOOH) are found in many enzymes in Nature, such as cytochrome P450, horse radish peroxidase and nitric oxide synthase, just to name a few. There are also examples of nonheme metal-oxygen utilizing enzymes, such as naphthalene dioxygenase, homoprotocatechuate 2,3-dioxygenase and taurine:α-ketoglutarate dioxygenase. These compounds catalyze common and essential reactions such as hydroxylation, epoxidation, desaturation and sulfoxidation. A given approach to understand the fundamentals of the reactions these compounds catalyze is to synthesize model systems. Our lab routinely produces and investigates the reactivities of such compounds, and this talk will give an overview of the theoretical calculations done in this area, in order to gain more insights than just experiments only could give.

CBC SEMINAR ANNOUNCEMENT

Dr Kyung-Bin Cho
Ewha Womans University, Korea

Synthetic Nonheme Metal-Oxygen Catalysts by Density Functional Theory:
These Can Be Versatile too

Date: 26th February 2013 (Tuesday)
Time: 1:30pm – 3:00pm
Venue: NTU SPMS CBC Building Level 2, Conference Room
Host: Asst Professor Hajime Hirao