

Predicting Activation Barrier, Reduction Potential and Fluorescence using Molecular Electrostatic Potential for Organic and Organometallic Systems

Bai Anjali[†]

Pusan National University

(anjaliamutha@gmail.com[†])

Chemical reactivity prediction with the help of computational chemistry is extremely important in predicting the perturbations, which stabilize or destabilize the molecule. The study explains that the molecular electrostatic potential (MESP) can be used as a powerful chemical reactivity descriptor by taking a variety of industrially important chemical systems as examples. A MESP based investigation using density functional theory (DFT) is carried out to predict the reduction potentials (E^0) of hydrogen evolution mononuclear cobalt electrocatalysts and Fischer chromium complexes. Also, the influence of mono- and multiple substituent effect on E^0 values of 1,3,6-triphenyl fulvenes is investigated using MESP. The absorption and fluorescence of a series of tris (8-hydroxyquinolino) M(III) complexes of aluminium, gallium and indium are presented where the MESP exhibited excellent correlations with the stokes shift values. A mechanistic interpretation of the oxidative addition of aryl halides to Pd(0) solely based on the MESP at the Pd center is established.