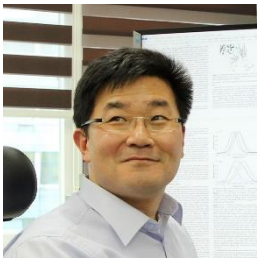
IBS Center for Multidimensional Carbon Materials

Special Seminar



Prof. Mu-Hyun BAIK

Dept. of Chemistry, KAIST
IBS Center for Catalytic Hydrocarbon Functionalizations
Daejeon, Korea

Can Computer Models Predict Complex Chemical Reactions?

November 1 **Wednesday, 2 PM**	Bldg. 101 Seminar Room 101

Computational molecular modeling has become an important tool of inquiry over the course of the last two decades. Its main use is to rationalize experimental observations that are often difficult to understand without a precise proposal for the structure of reaction intermediates that give rise to the observed properties. Whereas the power of computer models in locating and characterizing these intermediates has been well demonstrated, it is not at all clear that we can use computer models in a predictive fashion where unanticipated chemical reactions can be identified in the computer first or a set of simple experiments can be interpreted in a novel way using a computer model. In this presentation, I will discuss strategies for using computer models of catalytic chemical reactions in a predictive fashion to design new reactions.

Efforts to use precise models of reactive chemistry and overcome the bottlenecks of the standard workflow in chemical research led to new ways of more precisely controlling chemical reactions employing electrodes as functional groups with adjustable inductive effects. In this talk, I will discuss my vision about how novel catalytic processes can be developed fully exploiting precise computer models and the newly developed experimental techniques we have explored in the recent past. The ultimate goal is to create a new workflow of discovery that incorporates a more systematic exploration of the chemical reaction space.