NANYANG TECHNOLOGICAL UNIVERSITY

CBC SEMINAR ANNOUNCEMENT

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Systematic determination of complex reaction mechanisms

Transition metal catalysis is an efficient way to perform catalytic reactions in a controlled and a selective fashion. Quantitative details of mechanisms and selectivity of catalytic reactions are very important for the development of more efficient catalysis. These properties are however difficult to characterize from experimental studies alone, and therefore computational chemistry becomes critical.[1,2] The traditional computational methods for the study of potential energy surfaces (ground or excited states) require manual trial-and-error and guess-and-check processes. However, this strategy may miss some important or unexpected reaction paths. Therefore, new computational methods for comprehensive and systematic study of potential energy surfaces are crucial. In this direction, the artificial force induced reaction (AFIR) method is very useful.[3,4] The AFIR method determines equilibrium structures and subsequent reaction paths systematically, and therefore comprehensive description of the reaction mechanism and selectivity can be achieved.

I present mechanistic puzzles in transition metal-catalyzed aziridination,[5-7] where minimum energy seam crossing points between the singlet and triplet potential energy surfaces control the selectivity. Also, I will discuss AFIR applications that targeted the selectivity-determining step of transition metal catalyzed asymmetric carbon-carbon[8] and carbon-boron[9,10] bond formation reactions. My computational studies offer important mechanistic insights to develop broadly applicable catalytic reactions for potential applications in industry and academia.

References

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Date:	**8th August 2017 (Tuesday)**
Time:	**10:00am – 11:30am**
Venue:	**SPMS Research & Graduate Studies Office Conference Room**
Host:	**Professor Tan Choon Hong**