NANYANG TECHNOLOGICAL UNIVERSITY

CBC SEMINAR ANNOUNCEMENT

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Progresses and Difficulties the Modeling of Enzymatic Reactions

In this talk I will summarize the problems which we have been facing when we try to predict the catalytic mechanism of an enzymatic reaction. There is no obvious solution for most of them and there is no consensus about the approximations that should be made. The most important unsolved aspects are the appropriate Hamiltonian to be used, the dimension of the molecular model of the enzyme and substrate, and the extension in which the sampling of the conformational space should be carried out. The origin of the difficulties lies in the range of timescales that the enzymatic motion spans, and the long range of the interatomic interactions that act specifically to differentially stabilize the stationary species found along the potential energy surface.
The approximations that we have been carrying out will be presented and discussed. Our studies in enzymes such as Ribonucleotide Reductase, beta-galactosidase and farnesyltransferanse, among others, will illustrate the concepts. A comparison with other possible solutions will also be made.

Date:	**29th May 2012 (Tuesday)**
Time:	**11:00am – 12:30pm**
Venue:	**NTU SPMS CBC Building Level 2, Conference Room**
Host:	**Asst Professor Hajime Hirao**