University of Minnesota
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Department of Chemistry

Special Seminar

3:30 p.m. Monday, November 4 • 402 Walter Library

Professor

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Selectivity Modeling in Asymmetric Catalysis

Research interests: combination of experimental end computational techniques to elucidate the reaction mechanisms of organic transformations catalyzed by transition metal complexes.

Website:
http://www.gu.se/ViewPage.action?siteNodeId=537805&languageId=100001&contentId=-1

Abstract

Computational predictions of reaction selectivity can be a very useful tool for designing better synthetic methods, and in particular more selective catalysts. From a modeling perspective, the straightforward method is to calculate the reaction barriers to each possible product, and obtain the selectivity as the ratio of the rates to the products. For asymmetric selectivity, the problem can be simplified to inspection of transition states only, since the starting materials are identical for all paths. The high similarity between the different paths will reduce the effect of any systematic error in the theoretical model, allowing very high accuracy in the predictions. However, the major obstacle to true predictions is the need to find the best possible path to each product, requiring a global search through all possible conformations of the transition states. We have developed a method based on extrapolating model quantum systems through a molecular mechanics full size model (Q2MM). Our method gives unprecedented accuracies, and allows us to evaluate millions of paths per day on commodity workstations. The talk will give an overview of the development of the method from 1997 onwards, with examples from several metal-catalyzed processes.

Host: Professor Christopher Cramer