Computer Assisted Design of New Catalytic Reactions: Catalytic Borylation of Methane and Other Reactions

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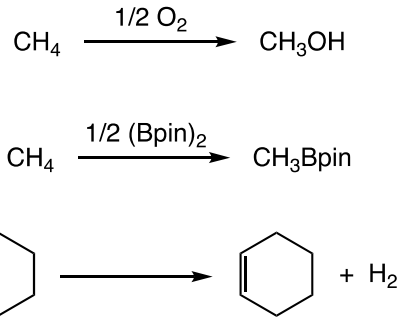
Computational molecular modeling has become a standard tool of mechanistic inquiry in the last decade. When combined with traditional experimental techniques, theoretical studies can be extremely powerful and deliver a detailed understanding of complex reactions and in some cases, be used as a predictive tool. In this talk, I will highlight three examples of such integrated studies where very challenging catalytic C–H activation reactions were thoroughly investigated. Nature has chosen to use iron to design a catalyst, methane monooxygenase, for the conversion of methane into biomass in methanotrophic bacteria. In synthetic organic chemistry, iridium is a metal of choice for developing a high-performance catalyst. And recently, we were able to show that titanium can be used to catalytically dehydrogenate alkanes. In all cases, C–H bonds that are very difficult to activate are broken at very mild conditions. In this presentation, I will highlight how different features of the metal-complexes are being utilized to accomplish these challenging transformations.



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