SS03-1 **ONIOM theoretical studies of chemical reactions in protein and organometallic catalytic reactions**

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Theoretical/computational chemistry has made a large advances in the last decades and has reached the stage where it can make highly accurate calculations and theoretical predictions for many chemical problems of relatively simple molecular systems. The main stream of chemistry has shifted toward complex molecular systems, and it has become necessary to develop theoretical methods for high-accuracy simulations of complex molecular systems in order to make theoretical predictions for new chemical materials and phenomena, It is still impossible to perform highly accurate ab initio simulations for complex molecular systems containing thousands of atoms for a long time (~10^6 calculations) and the development of more efficient hybrid methods combining different levels of computational methods is highly desirable. We have been working toward this goal and in the present lecture I will discuss some examples of such studies on the mechanism of homogenous catalysis by organometallic compounds and on the mechanisms of chemical reactions in protein (enzyme reactions) using the ONIOM method.