Simulating Heterogeneous Catalysis for Energy- and Environment-Related Applications

ABSTRACT: Sustainable development of the world requires efficient processes and materials that can convert sustainable resources into fuels and chemicals. The design and development of robust heterogeneous catalysts for practical applications have been hindered by our limited understanding of the underlying physical/chemical processes that govern the catalytic transformations. Recent advances in DFT-based electronic methods, molecular simulations and the availability of computing power provide unprecedented ability to track these molecular transformations and how they proceed at specific sites and within particular environments. Over the past decades, we have the opportunities of applying these methods in studies of catalytic materials and processes related to CO$_2$ and CH$_4$ activation and conversion and other application. In this talk, I will present selected results and discuss their implication to practical applications.