Catalyst Design from First-Principles Calculation
(제일원리 계산을 활용한 촉매 설계)

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One of the major barriers to their commercialization in energy conversion is the high cost and low efficiency of catalysts in running the energy conversion devices. Thus, there exists great interest in developing alternative catalytic materials. The essential part in the development and optimization of high-performance catalysts for energy applications is to properly tailor the physical and chemical properties of catalysts. However, a detailed understanding of how to control the properties of such catalysts is still lacking, despite its importance in designing and developing novel and cost effective catalysts. This is in large part due to the difficulty of direct characterization. Alternatively, quantum mechanics-based computational approaches (First-Principles) have emerged as the powerful and flexible means to unravel the fundamental principles of catalysts, which may allow the new finding of the breakthrough catalysts. In this talk, I will present the recent studies on the First-Principles design of catalytic materials for energy applications.