Revealing the Origin of High Activity of Rhodium for Catalytic Dehydrogenation of Light Alkanes Using Kinetic Monte Carlo Simulation

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As the recent shale gas boom has provided an attractive feedstock of light alkanes (C1~C3), global demand for a commercial light alkane dehydrogenation (LAD) catalyst is ever increasing for the efficient production of propylene and ethylene. Several studies on rhodium (Rh)-based catalysts showed high activity and moderate selectivity comparable to the conventional Pt based catalyst. However, the atomic nature of the high catalytic efficiency of Rh is still elusive due to the lack of deep understanding on the complex LAD reaction network. Herein, a DFT-based kinetic Monte Carlo (kMC) simulation is performed on Rh (111) surface for the two major LAD reactions, propane dehydrogenation (PDH) and ethane dehydrogenation (EDH). By performing kinetic analysis using reaction conditions, the rate determining reaction steps of dehydrogenation, cracking and coke formation are identified. Based on our results, we proposed the optimal reaction conditions for selective and active LAD, and proposed strategies to minimize the coke formation. Our theoretical analysis will pave the way to design a highly active and coke resistant Rh-based catalyst for LAD.