Dehydrogenation of perhydro-dibenzyltoluene over Pt-based subsurface alloys : A density functional theory

Zhou Jingwen, 강성구†
울산대학교
(sgkang@mail.ulsan.ac.kr†)

We systematically explored the dehydrogenation process of perhydro-dibenzyltoluene (H18-DBT) over Pt(111) and Pt-based subsurface alloys, such as Pt/Pd/Pt(111), Pt/Cu/Pt (111), and Pt/Ni/Pt(111) using DFT calculations. The adsorption strength of H18-DBT on each system and the relevant charge transfer between H18-DBT and the catalysts were investigated. More importantly, the performance of each catalyst was compared to each other through free energy diagram analysis. Our study will provide a theoretical guidance for designing highly active Pt-based catalysts for dehydrogenation of liquid organic hydrogen carriers (LOHC) systems.