COMBINED IN SITU XAS AND DFT STUDIES ON THE ROLE OF PT IN ZEOLITE-SUPPORTED METAL CATALYSTS FOR SELECTIVE N-HEXANE ISOMERIZATION

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In this study, we used several in situ, and spectroscopy analyses to investigate the roles of platinum (Pt) in zeolite-supported Pt catalysts for selective n-alkane isomerization. Catalytic testing at 300 and 450 ℃ used hydrogen gas as both reactant and carrier. Typically, HY zeolites have proved to be active hydrocarbon cracking catalysts. The particular challenge is to find an effective catalyst, which favors the isomerization of n-alkanes without too much cracking. In this work, adding Pt atoms to HY zeolite provides an enhanced multifunctional catalyst for converting *n*-alkanes to branched hydrocarbons. To understand the effect of Pt, we further investigated the reaction mechanism of n-hexane isomerization to 2 methylpentane (2MP) and 3-methylpentane (3MP) by DFT simulations, using a cluster of 30T HY zeolite modeled through B3LYP+3D calculations. We found that, at 450 ℃, the isomerization on Pt-HY gives higher cracking products. Decreasing temperature to 300 ℃ yielded greater selectivity of branched hydrocarbons. In addition, DFT calculations demonstrate that the 2MP production via route A1 (C3–C4 bond activation) and a rate-determining step of 0.97 eV proved more thermodynamically and kinetically favorable than the 3MP product. This agrees well with our experimental observations. Consequently, the presence of Pt on the HY zeolite plays an essential role in both C–C forming and breaking. Finally, the Pt HY zeolite is an efficient catalyst for petroleum production, improving the octane number for catalytic performance and product selectivity by isomerizing straight-chain alkanes to their branched chain isomers.

Keywords: Hexane isomerization; Pt-HY zeolite; *In situ* CO_2-TPD; DFT; *In situ* XAS