

Abstract Submitted
for the OSS15 Meeting of
The American Physical Society

Stability Analysis of Metal Oxide Catalyst Using Computational

Method KWANGJIN AN, Department of Chemistry, University of California, Berkeley, RICHARD KYUNG, Choice Research Group, TERRI T. HAHN, Choice Research Group (James Madison HS), GABOR A. SOMORJAI, Department of Chemistry, University of California, Berkeley — To actualize green energy in the hydrogenation/dehydrogenation reactions, study on the mechanisms of selectivity and specific analysis on the molecular stability of the product are required. Porous oxide supports and metal nanoparticles can increase catalytic selectivity to obtain desirable products. In this experiment, n-Hexane isomerization as a multipath reaction was carried out over 2.7 nm Pt nanoparticles on five kinds of oxide supports over the temperature range of 240–360 °C in 140 Torr n-hexane and 620 Torr H₂. Under these reaction conditions, multiple products were generated through four distinct reaction pathways: branched isomers via isomerization, methylcyclopentane and cyclohexane via cyclization, benzene via dehydrogenation of cyclohexane (aromatization), and cracked hydrocarbons with short chains (C1–C5) via hydrogenolysis. For the stability analysis, the chemical catalytic efficiency and physical activities of proposed metal oxide compounds are modeled and analyzed using computational simulations. The oxide compounds' chemical and physical properties, such as repulsive forces, electron structures, and bond strengths are studied using computational quantum mechanical modelling method.

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Date submitted: 21 Feb 2015

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