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Mechanistic Study of Ethanol Conversion into Butadiene over Silver promoted Zirconia Catalysts

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GRAPHICAL ABSTRACT

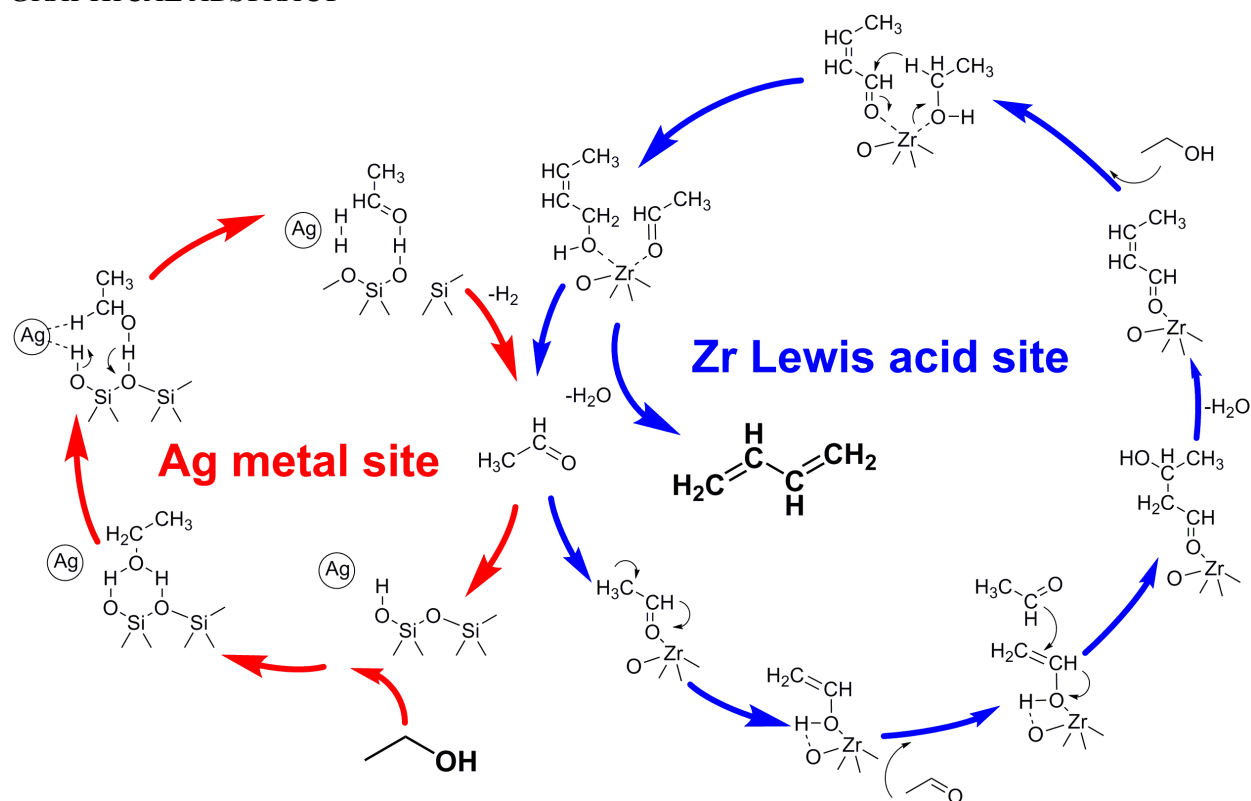


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Highlights

Combined application of kinetic measurements, SSITKA and deuterium tracing techniques allowed to elucidate the mechanism of the key steps of butadiene synthesis over silver promoted zirconia supported catalysts, including ethanol dehydrogenation, acetaldehyde aldol condensation, and crotonaldehyde reduction with ethanol, and to determine the rate-limiting step of the process. We show for the first time that butadiene synthesis involves two independent catalytic cycles: i) dehydrogenation of ethanol into acetaldehyde over metal sites, and ii) acetaldehyde/ethanol transformation into butadiene over Lewis acidic sites. The proposed

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