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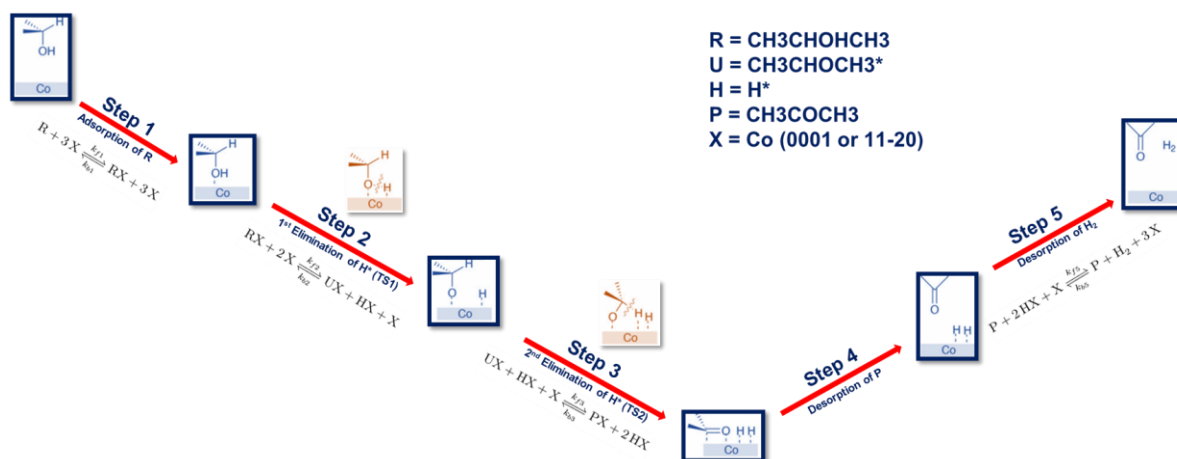
# Engineering the Performance of Cobalt in the Dehydrogenation of Isopropanol into Acetone via the Use of Multiscale Approach

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This study was geared towards the computational design of an effective and efficient heterogeneous catalyst for the biomass conversion process by exploring cobalt metal performance to catalyze the dehydrogenation of isopropanol into acetone to understand the surface view that best influences the kinetics of the reaction. The study was done via multiscale approaches combining DFT and kinetic modeling, where steps and states influencing the kinetics were identified, and the best surface of the catalyst that best promotes the reaction rate was investigated. Findings from the study would provide better insight into the role of the catalyst surface views, including the role played by ligands in altering the kinetics of reactions.



**Figure 1** – Schematic Diagram for the Dehydrogenation of Isopropanol into Acetone

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