Exploring the steam reformation process of alkanes and fuel alcohols on metal catalysts

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We have theoretically modeled the reaction pathway from small organic molecules to synthesis gas on select metal atom catalyst. Using methanol as the reactant, the lowest energy intermediate along the reaction path is the insertion product H-M-OCH_3 (M = V and Fe). Starting with ethanol, as the reactant the lowest energy isomer is also the H-Fe-OCH_2CH_3 insertion product(shown below). We are in the process of building an experimental apparatus capable of preparing and isolating these intermediates in large enough quantities to study with infrared spectroscopy (right). It is expected that we will be able to synthesize the theoretically predicted lowest energy intermediates.