A theoretical and experimental spectroscopy study on methanol and ethanol conversion over H-SAPO-34

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The elucidation of the structure-activity relation of zeolites or zeotype materials remains very challenging. Recent advances in both theoretical and experimental techniques provide new opportunities to study these complex materials and any catalytic reaction occurring inside. In order to establish new active reaction routes, the knowledge of formed intermediates is crucial. The characterization of such intermediates can be done using a variety of spectroscopic techniques. In this contribution, methanol and ethanol conversion over H-SAPO-34 is investigated using IR and UV-VIS measurements.

Calculated adsorption enthalpies of methanol and ethanol in a large SAPO 44T finite cluster show the stronger adsorption of the larger alcohol by 14 kJ mol^{-1}. Dispersion contributions are found to be crucial. IR spectra are calculated for the clusters containing the adsorbed alcohols and matched with experimental data. In addition, the cluster is also loaded with singly methylated cationic hydrocarbons as these are representative reaction intermediates. A detailed normal mode analysis is performed, enabling to separate the framework-guest contributions. Based on the computed data in situ DRIFT experimental peaks could be assigned. Finally, contemporary DFT functionals such as CAM-B3LYP seem promising to compute gas phase UV-VIS spectra.