FIRST-PRINCIPLES STUDY OF INFRARED AND RAMAN SPECTRA OF INTERMEDIATES IN ETHANOL CONVERSION TO ETHYL ACETATE AND HYDROGEN

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Ethanol dehydrogenation dimerization to form ethyl acetate (EA) and hydrogen is, in principle, the best atomically economic reaction and is also considered to be an environmentallly friendly process in EA synthesis. Even though the copper-based catalysts have been utilized as commercial catalysts they still have some disadvantages such as low productivity and difficult separation from the by-products. Density functional theory was used to investigate the ethanol dehydrogenation dimerization over Cu(111) catalyst. In this work, we calculated and analysed the reaction network on Cu(111) along different dehydrogenation pathways. In addition, to improve the performance of Cu-based catalyst, we investigated the activities over $Cu_3Pt(111)$ and $Cu_3Pd(111)$. By comparsion, the introduction of Pt or Pd is beneficial for the improvement of catalytic activity. The analysis of density of eletronic states was used to explain how these electron transfers were proceeded over different catalysts. Through calculating the entire frequencies of each intermediate, the Infrared and Raman spectra for each intermediate were predicted that will be useful to experimental detection of intermediates.