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Rh-based Catalysts for the Ethanol Conversion as an Alternative Fuel Additive JAEWON YOU , KMLA, JEREMIAH YOON, The Gunnery, CHUNG UN LEE, Choice Research Group — Oil is definitely the most important of all the energy sources and fossil fuels have accounted for the most of the energy produced. Ethanol is not an efficient fuel, but it is well-known to act as a great fuel additive. To improve fuel efficiency, researchers have discovered ways to add ethanol to gasoline combustion. Catalytic oxidation reactions are crucial for chemical synthesis in pharmaceutical and petrochemicals industries. Rhodium(Rh) is a major component of industrial catalytic systems, and it is found as free metal, along with nickel and copper deposits. The focus of this project is the study of catalysts for the conversion of ethane to ethanol that can be used as a fuel additive: Rhodium dichlorine monoxide($RhCl_2O$), Rhodium oxide(RhO), and Rhodium hypochlorite(RhClO). The catalytic efficiency of those compounds will be modeled and explained based on the compound's electron structure and how the catalytic efficiency could be improved even more by forcing the catalyst to react with ethane in different ways. Computational chemistry will be used to find the best catalyst for the conversion of ethanol, which will advocate the ethanol economy.

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