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Enhancements of Catalytic Behavior Using Metal Oxides JIHYUN HWANG, HAEUN LIM, JONATHAN KIM, Choice Research Group — Many studies have shown that the enhancements of catalytic behavior were produced due to the role of the oxide-metal interface, which plays a crucial role in catalytic process industry. Increase of surface oxide-metal interface increases the ability of individual molecules to attract each other and causes weaker intermolecular force. The properties of an atom such as its momentum, position, and energy level are defined by the electron structure, and the catalytic efficiency of a compound depends on its electron structure as well. This project aims to determine the catalyzing ability of Rhenium compounds using a computational chemistry method, also using programs such as Avogadro and Chemcraft, in an effort to discover the optimal method and to compute the measures of catalytic ability. Density Functional Theory (DFT), a computational chemistry, is used in order to model the electron properties of the compound. Gamess is a program that allows performing such computations for a compound. It takes an input file of a defined format and converts it into an output describing the molecule and the reaction. This program shows the optimized geometry energy levels and fully determines the theoretical values of the structures atomic properties.

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