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Study on the Stability of Catalysts for Alcohol Conversion as a New Energy Source JEONG H. (PETER) YOON, SUYEONG HAN, LUTHER LU, RICHARD KYUNG, CRG(Choice Research Group) — In this paper, the catalyzing ability of Palladium and Rhodium compounds as catalysts using computational chemistry method was carried out. Programs such as Gamess and Chemcraft were used in an effort to compute the measures of catalytic ability. This paper focused on studying Palladium and Rhodium compounds as catalysts for the conversion of methane to methanol as a new energy source. The catalytic efficiencies of XCl_2O, XClO, and XClO (X: Palladium and Rhodium) were modeled and explained based on the compound's electron structure, resonances, and number of iterations to converge. Also this paper shows how the catalytic efficiency could be improved even more by forcing the catalyst to react with methane in different ways. In order to model the electron properties of the compound, Density Functional Theory (DFT) methods of computational chemistry was used.

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