

Abstract Submitted
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Ti-based Catalysts for the Methanol Conversion as an Alternative Energy Source DOWOON YOON, BYEONGYEON CHO, RICHARD KYUNG, Choice Research Group — The United States has more natural gas than petroleum. If we are able to exploit that abundance by converting it to methanol, then the dependency on foreign fuel would be reduced. Prior research results have been controversial regarding the efficiencies of each catalyst. However, the contradictory results are due to inconsistencies of the theoretical and computational models, which we reconcile in our model. Places for oil production are becoming more and more costly, therefore, alternatives need to be considered before they run out. At the end of the study, the catalytic efficiency of TiCl_2O , TiO , and TiClO 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 methane in different ways. The Density Functional Theory will be used to prove that TiCl_2O is the best catalyst for the conversion of methanol, which will advocate the methanol economy.

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