Inorganic Materials & catalysis

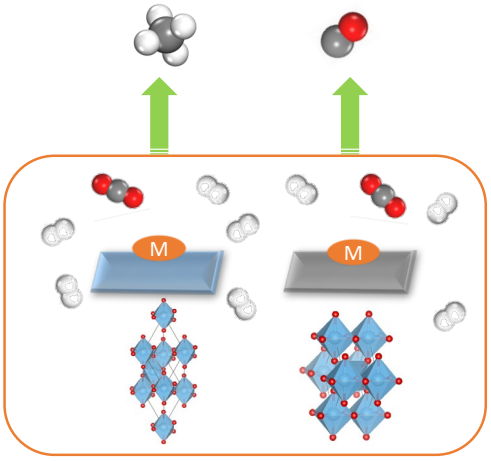
Research Project – Emiel Hensen/Lulu Chen

IMC
INORGANIC MATERIALS & CATALYSIS

CO_2 methanation on Titanium-based catalyst

Background

Conversion of CO_2 to valuable products has been attractive to chemist. CO_2 methanation (Sabatier reaction), which convert CO_2 and H_2 to CH_4 and H_2O, has been crucial for reducing global CO_2 emission. It is favored thermodynamic at low temperature but limited kinetically because of the high stability of CO_2. The catalysts widely studied in literatures are based on Ni, Ru, Rh, Pd supported different supports such as CeO_2, TiO_2, Al_2O_3, ZnO_2, SiO_2, ZrO_2 metal carbide and carbon materials. CO_2 methanation over supported nickel catalysts attracts an increasing attention due to their higher cost performance. Redox supports such as TiO_2 and CeO_2 show better catalytic performance than non-redox supports. The activity and selectivity of catalysts are influenced by several factors, such as the morphology, the size and oxidation state and supported metals, strong metal support interaction. The product selectivity can be tuned from CO to methane via phase transition of the anatase to the rutile.[1] On Titanium-based catalyst, SMSI induce a titania overlayer around Ni cluster, which significantly suppressed catalytic activity.[2] However, Zhang and co-workers suggested that the activity depends on the extent of encapsulation of metal particles by TiO_x layer.[3]



In this project, we aim at investigating CO_2 methanation mechanism on Ni supported different phase of TiO_2 to give an explanation of the effect of different phases. By loading a TiO_2 cluster on Ni (111) surface, we will investigate the effect of partial encapsulation of TiO_2.

Techniques used:

1. Perform DFT calculations to explore reaction mechanisms.
2. Develop microkinetic modeling simulations to investigate the reaction mechanisms.

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[1] Li, Wenhui, et al. CO_2 hydrogenation on unpromoted and M-promoted Co/TiO_2 catalysts (M= Zr, K, Cs): effects of crystal phase of supports and metal–support interaction on tuning product distribution. ACS Catalysis 9.4 (2019): 2739-2751.
[2] Li, Jian, et al. Enhanced CO_2 methanation activity of Ni/anatase catalyst by tuning strong metal–support interactions. ACS Catalysis 9.7 (2019): 6342-6348.
[3] Xu, Jinghua, et al. Influence of pretreatment temperature on catalytic performance of rutile TiO_2-supported ruthenium catalyst in CO_2 methanation. Journal of Catalysis 333 (2016): 227-237.