



## Reaction mechanism for NO decomposition on oxotitanium porphyrin with $\text{NH}_3$ -selective catalytic reduction: A DFT study

Nitric oxide (NO), one of the pollutant gases released from exhaust and industrial process, plays a major role in undesired effects such as greenhouse effect. Commercial catalysts for  $\text{NH}_3$ -selective catalytic reduction (SCR) of NO are extensively used in removal of NO. However, these catalysts may give some drawbacks including toxicity at high temperature range. An alternative catalyst for  $\text{NH}_3$ -SCR is paid attention on metal-porphyrins for NO conversion to  $\text{N}_2$ . The reaction mechanism of NO decomposition with  $\text{NH}_3$ -SCR to environmental friendly products (e.g.  $\text{N}_2$ ,  $\text{H}_2\text{O}$ ) of oxotitanium-porphyrin catalyst (TiO-Por) has been systematically investigated by means of density functional theory (DFT) calculations with M06L functional to explore the potential use of this catalyst. In this study, the mechanistic cycle of NO decomposition with  $\text{NH}_3$ -SCR is proposed in four steps: 1) NO adsorption, 2) oxidation of  $\text{NH}_3$ , 3) formation of  $\text{NHNOH}$  via  $\text{NH}_2$ -NO intermediate and 4)  $\text{NHNOH}$  decomposition. From our calculations, the N-H bond cleavage in the formation of the  $\text{NHNOH}$  intermediate is the rate determining step with the energy barrier ( $E_a$ ) of about 32 kcal/mol. The NO decomposition releases  $\text{N}_2$  and  $\text{H}_2\text{O}$  as the products, implying that the catalyst has high selectivity toward  $\text{N}_2$  with a small desorption energy of about 3 kcal/mol. In addition, the activation energy for  $\text{NH}_3$ -SCR of NO decomposition is lower than the reduction of NO over the commercial catalysts. The results suggest that TiO-Por is a potential catalyst for NO decomposition with  $\text{NH}_3$ -SCR.

### References

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**Primary author:** Dr DAENGNGERN, Rathawat (National Nanotechnology Center, NSTDA, 111 Thailand Science Park, Phahonyothin Road, Khlong Nueng, Khlong Luang, Pathum Thani 12120 Thailand)

**Presenter:** Dr DAENGNGERN, Rathawat (National Nanotechnology Center, NSTDA, 111 Thailand Science Park, Phahonyothin Road, Khlong Nueng, Khlong Luang, Pathum Thani 12120 Thailand)

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