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Reaction mechanism for NO decomposition on oxotitanium porphyrin with NH₃ 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 NH₃-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 NH₃-SCR is paid attention on metal-porphyrins for NO conversion to N₂. The reaction mechanism of NO decomposition with NH₃-SCR to environmental friendly products (e.g. N₂, H₂O) of oxotithanium-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 NH₃-SCR is proposed in four steps: 1) NO adsorption, 2) oxidation of NH₃, 3) formation of NHNOH via NH₂NO intermediate and 4) NHNOH decomposition. From our calculations, the N–H bond cleavage in the formation of the NHNOH intermediate is the rate determining step with the energy barrier (E_a) of about 32 kcal/mol. The NO decomposition releases N₂ and H₂O as the products, implying that the catalyst has high selectively toward N₂ with a small desorption energy of about 3 kcal/mol. In addition, the activation energy for NH₃-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 NH₃-SCR.

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