Organized by Endorsed by
8th IUPAC INTERNATIONAL CONFERENCE ON GREEN CHEMISTRY
9 - 14 September 2018, Shangri-La Hotel, Bangkok, Thailand

8th ICGC 2018 Session:

Facet dependent catalytic performances of anatase-TiO_2 toward selective catalytic reduction of NO with NH_3: A DFT-D study

Supawadee Namuangruk
National Nanotechnology Center (NANOTEC), National Science and Technology Development Agency, 111 Thailand Science Park, Pathum Thani 12120, Thailand
**E-mail: supwadee@nanotec.or.th*

Abstract: Recently we found that TiO_2 nanosheet exposed the (001) plane showed superior SCR performance to TiO_2 nanoparticles exposed the (101) plane. In this study, the deep understanding on the origin of the facet dependent catalytic performances are analyzed using the plane wave-based density functional theory method. The reaction mechanism of selective catalytic reduction of NO using NH_3 as a reducing agent (NH_3-SCR) on the (001) and (101) surfaces were comparatively investigated. The results clearly showed that the (001) surface has higher active site and higher surface energy resulting in a promising catalytic performance for the reduction of NO via NH_3-SCR validated by low activation energies of reactions compared with (101) surface. The surface-assisted mechanisms are predominant processes observed in the (001) plane. According to the most favorable pathway, the rate-determining steps of the reactions on the (001) and (101) surfaces are the NH_3 dissociation and the NH_2NO decomposition, respectively. The results agree well with the experimental observation that the active sites play a crucial role facilitating the NH_3-SCR of NO on anatase-TiO_2 (001) at low temperatures.

Keywords: NH_3-SCR, NO, anatase-TiO_2, DFT

Supawadee Namuangruk is a senior researcher in National Nanotechnology Center (NANOTEC), Thailand. She received her Ph.D. in chemistry from Kasetsart University in 2007 and then she did a postdoctoral research at Humboldt University, Germany in 2008. After five-year of research experience in NANOTEC, she has become a Team leader of Nanoscale simulation Laboratory since 2013. Her research interest is using first principle computational chemistry method to design and predict the properties of functional nanomaterials for applications in heterogeneous catalysis, dye-sensitized solar cells, adsorbents for heavy metals and volatile organic compounds.