第405回触媒科学研究所コロキウム

DFT investigation of H2S Desulfurization on Anatase TiO2 (001) Surface

Dr. Supawadee Namuangruk

(Group Leader, Nanoscale Simulation Laboratory, National Nanotechnology Center (NANOTEC), National Science and Technology Development Agency (NSTDA), Thailand)

2017年9月25日(月)15:00—16:00 創成科学研究棟 4階 セミナー室A

http://www.cat.hokudai.ac.jp/access.html

The complete reaction mechanism for the H2S desulfurization on anatase TiO2(001) surface was elucidated using the plane-wave based density functional theory method. The reaction started from the dissociative adsorption of H2S on the TiO2 surface. Subsequently, two competitive routes, the H2O and H2 formations, were laterally investigated. The activation barriers for the H2O formation are ranging from 11-13 kcal/mol, whereas those for the H2 formation are extremely high in the range of 67-87 kcal/mol. On the basis of the activation energy barriers, the results indicate that the anatase TiO2(001) is very active for the H2S desulfurization to produce H2O, resulting in the S-substitution at the O2c site of TiO2(001) surface. Electronic charge analyses indicate that the S doping into the TiO2 surface can enhance the photocatalytic activity of TiO2 by reducing its energy band gap. In addition, by comparison with other metal oxide catalysts such as TiO2(101), CeO2(111), CeO2(101), ZnO (1010) and 日 Fe2O3(0001), the TiO2(001) is found as the most promising catalyst for the H2S desulfurization.

【Dr. Supawadee Namuangruk】
Supawadee Namuangruk obtained her Ph.D. in Chemistry from Kasetsart University (2007). After that she joined the Nanoscale Simulation Laboratory (SIM lab) in NANOTEC. 2013-Present; she is a senior researcher and the team leader of SIM lab. Her research focus is in the fields of heterogeneous catalysis using periodic density functional theory and quantum chemical calculation.

問合せ先: 触媒科学研究所 長谷川淳也(hasegawa@cat.hokudai.ac.jp 011-706-9145)