可視光応答型光触媒材料としてのチタン酸窒化物の理論提案

Titanium Oxynitride as a Visible-light Photocatalyst

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Over the decades, impurity doping into TiO_2 is one of the hottest subjects in the research for realizing high-performance visible-light photocatalytic materials. Especially, N doping is one of the most successful methods to make TiO_2 visible-light-active. Importance of N is that the N 2*p* state redshifts the absorption, which is originally determined by the O 2*p* state. However, absorption of N-doped TiO_2 in the visible-light region is much weaker than that in the ultraviolet region. This should be because the concentration of N is limited in N-doped TiO_2. On the other hand, the system with the maximum N-concentration limit, TiN, is metallic because the valence number of Ti is +3 and an excess electron per Ti atom exists. Therefore, one needs to keep the valence number of Ti +4 in order to achieve the semiconducting system with high N concentration. In order to meet the requirement, we propose titanium oxynitride with the composition Ti_2N_2O. The structure of our proposed Ti_2N_2O is based on that of corundum-type Ti_2O_3. We investigate the electronic structure and the energetics of Ti_2N_2O within the framework of the density-functional theory (DFT). We find that the band gap of Ti_2N_2O is smaller than that of rutile TiO_2 and anatase TiO_2 by 0.79 eV and 1.04 eV, respectively. We also find that the band-gap reduction in Ti_2N_2O is achieved by upshift of the valence band maximum (Figure 1). Such a band structure is suitable for photocatalytic water decomposition. Finally, we conduct the energetic analysis on Ti_2N_2O and N-doped TiO_2. It is found that the energy per N atom required to form Ti_2N_2O from Ti_2O_3 is smaller than the impurity defect formation energy of N-doped TiO_2.

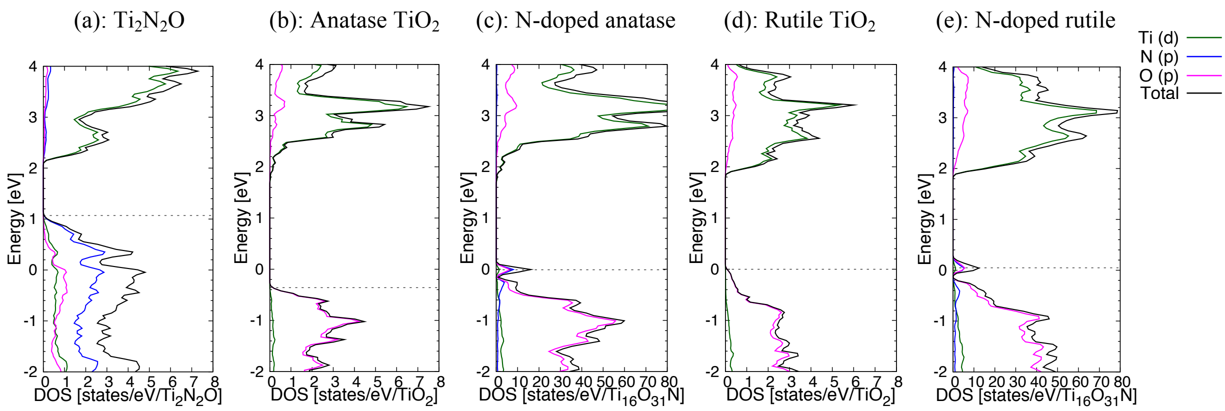

Figure 1: Total and projected density of states of Ti_2N_2O compared to those of anatase TiO_2, N-doped anatase, rutile TiO_2, and N-doped rutile.