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$_2$N$_2$O. The structure of our proposed Ti$_2$N$_2$O is based on that of corundum-type Ti$_2$O$_3$. We investigate the electronic structure and the energetics of Ti$_2$N$_2$O within the framework of the density-functional theory (DFT). We find that the band gap of Ti$_2$N$_2$O 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$_2$N$_2$O 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$_2$N$_2$O and N-doped TiO$_2$. It is found that the energy per N atom required to form Ti$_2$N$_2$O from Ti$_2$O$_3$ is smaller than the impurity defect formation energy of N-doped TiO$_2$.

![Figure 1](image-url)  
**Figure 1:** Total and projected density of states of Ti$_2$N$_2$O compared to those of anatase TiO$_2$, N-doped anatase, rutile TiO$_2$, and N-doped rutile.