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DFT-based Theoretical Calculation of Nb- and W-doped Anatase TiO_2 TAKAHIRO SUENAGA, HIDEYUKI KAMISAKA, HISAO NAKAMURA, KOICHI YAMASHITA, The University of Tokyo — The structure and electronic states in the Nb-doped TiO_2 (TNO) and W-doped TiO_2(TWO) in anatase phase were investigated from the first-principle using DFT-based band structure method. In addition to the cases where the dopant substituting a Ti atom, cells containing a dopant (M_{Ti}; M = Nb, W) and an oxygen vacancy (V_O) were calculated in order to clarify the role of the oxygen vacancy in the system. Furthermore, cells containing two dopants and an oxygen vacancy ($2M_{Ti}$–V_O), and cells with a dopant and two oxygen vacancies (M_{Ti}–$2V_O$) were calculated. Energetically stable structures were found among the sampled $2W_{Ti}$–V_O and W_{Ti}–$2V_O$ cells, while the corresponding structures in TNO did not show any significant energy stabilization. Impurity states were found in the stable $2W_{Ti}$–V_O and W_{Ti}–$2V_O$ structures, and an approach of the two W_{Ti} atoms was observed in the former. The present results rationalize the lower electronic conductivity of TWO than that of TNO, and suggest possible formation of complex structures consisting of the W_{Ti} dopants and the oxygen vacancies.

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