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DFT-based Theoretical Calculation of Nb- and W-doped Anatase **TiO**<sup>2</sup> 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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