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DFT-based first-principle calculation of Nb- and W-doped anatase TiO_2: Its stoichiometry and the formation of impurity complexes[1] HIDEYUKI KAMISAKA, TAKAHIRO SUENAGA, HISAO NAKAMURA, KOICHI YAMASHITA, The University of Tokyo — The structure and electronic states of Nb-doped anatase TiO_2 (TNO), a novel transparent conducting oxide, were calculated from the first-principle. Emphasis was put on the importance of non-stoichiometry of the system, because the high electronic conductivity emerges only in samples fabricated under a strong reductive atmosphere, and O_2 gas annealing deteriorates the conductivity. The non-stoichiometric system was modeled with periodic unit cells containing several combinations of Nb dopants, oxygen vacancies, and interstitial oxygen atom. From the result, experimental measurements of Nb 3d XPS signal and the effect of O_2 gas annealing were rationalized. Some complex structures exhibit strong energy stabilization. These structures might be a constitutive part of the electronic pathway. Similar calculations were performed for W-doped anatase TiO_2, and the difference from TNO was discussed.

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