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DFT-based first-principle calculation of the carrier activation ratio in the F-doped anatase TiO_2 and the thermodynamic analysis of the formation of $TiOF_2$ phase HIDEYUKI KAMISAKA, NANAKO MIZUGUCHI, KOICHI YAMASHITA, TETSUYA HASEGAWA, The University of Tokyo — The F-doped anatase TiO_2 (FTO) could be an alternative transparent conductive oxide, but the experimentalists have reported low carrier activation ratio of 20 - 30%, and that the formation of $TiOF_2$ hampers its production when using the PLD method. We investigated this system using the standard DFT-based band structure method. The PBE functional was adapted with the Hubburd +U terms. The value of +U parameters was adjusted to meet the generalized Koopman's theorem (gKT). We found that the formation energy of F_O (F dopant substituting O) and F_O^+ is quite close to each other, and the two crosses when the Fermi level is slightly above the conduction band minimum. Combining the Burstein-Moss effect and this crossing of the formation energies, a simple statistical analysis was made. The calculated activation ratio was about 10% - 32%, which agreed with the experimental data. The free energies of bulk TiO_2, 3% FTO, 6% FTO and $TiOF_2$ were compared using the DFT result. Contributions from the distribution entropy of the anions, lattice vibrations, free energy of conductive electrons, and the entropy from the spin state of trapped electrons was considered with relevant approximations. We found that the free energy of TiO_2, 3% FTO, and $TiOF_2$ come close to each other under the condition of T=800K and $P(O_2) = 10^{-5}$ Torr, which coincides the experimental report.

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