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A hybrid density functional study on energetics of native defects in anatase TiO_2 ADISAK BOONCHUN, National Institute for Materials Science (NIMS), Japan, PAKPOOM REUNCHAN, Kasetsart University, Thailand, NAOTO UMEZAWA, (1) National Institute for Materials Science (NIMS), Japan (2) JST PRESTO (3) TU-NIMS Joint Research Center, Tianjin University, China, JINHUA YE, (1) National Institute for Materials Science (NIMS), Japan (2) WPI-MANA (3) TU-NIMS Joint Research Center, Tianjin University, China — The energetics and electronic structures of native defects in anatase TiO_2 have been studied by means of hybrid density-functional calculations. Here, we show that oxygen vacancy (V_O) and titanium interstitial (Ti_i) are both shallow donors and are likely to form with a substantial concentration in an oxygen poor condition. While titanium vacancies (V_{Ti}) is a deep acceptor. The charge neutrality showed that Fermi level is pinned at the conduction band minimum in good agreement with the common observations of n-type conductivity in a reduced TiO_2. Self-trap hole (O_O) states are localized at oxygen anions. On the other hand the self-trapped electron (Ti_{Ti}) cannot be produced in the bulk. Although, Ti_i is the strongest candidate for the unintentional n-type conductivity owning to its low formation energy, we show that the post-growth of V_O in anatase is also possible under annealing temperature and pressure.

Adisak Boonchun
National Institute for Materials Science (NIMS), Japan

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