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.