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**Synthesis conditions and electronic structures of heavily N-doped TiO<sub>2</sub>** YUTA AOKI, Tokyo Institute of Technology, NAOTO UMEZAWA, National Institute for Materials Science, SUSUMU SAITO, Tokyo Institute of Technology — TiO<sub>2</sub> has drawn a lot of attention for its notable photocatalytic properties. Unfortunately, however, only a small portion of solar spectrum is utilized for photocatalytic activities of TiO<sub>2</sub> because of its wide band gap. To harvest solar energy more efficiently, TiO<sub>2</sub> must be sensitized under the irradiation of visible light which accounts for nearly 50 % of solar light reaching ground surface. Although N-doped TiO<sub>2</sub> is a well-known visible-light driven photocatalyst, its photoabsorption cross section is still limited. In order to enhance visible-light absorption, high-concentration doping of N should be a promising solution. Here, we propose the synthesis conditions of heavily N-doped TiO<sub>2</sub> both for rutile and anatase structures based on the density-functional theory. We use supercell models with several different N concentrations to clarify the concentration dependence of the synthesis conditions. To discuss the synthesis conditions, we enforce a constraint to avoid the precipitation of other compounds, e.g. TiN, TiO, Ti<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>, during the synthesis of heavily N-doped TiO<sub>2</sub>, which is described as a set of inequalities with respect to chemical potentials of N and O ( $\mu_N$  and  $\mu_O$ ) The results show that  $\mu_N$  must be larger than zero, which should be the upper limit for chemical potentials, in order for heavily N-doped TiO<sub>2</sub> to deposit stably. This means that high-concentration N doping is energetically difficult to be realized. Also, we will discuss the local arrangement of N atoms in connection with O vacancies and the electronic structures of examined models.

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