Formation energy of charge states of nitrogen and oxygen vacancies in anatase TiO_2: An ab initio study

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Electronic and structural properties of several charge states of interstitial (Ni) and substitutional (Ns) nitrogen and oxygen vacancies (V_O) into anatase TiO_2 were studied through density functional theory calculations.
The formation energies indicate that different charged states happen in the range of allow edelectronic chemical potential, *μe*. ForN-doping,neutral and positively charged states occur at μe near the valence band top, namely N^0_s, N^+_s and N^{2+}_i, while negatively charged states occur at μe near the conduction band bottom, N^-_s and N^-_i.
N_i is energetically more stable than N_s and always has a negative formation energy. The presence of oxygen vacancies would facilite the formation of N^-_s because the defects levels associated to V_O can pin the Fermi level close to the bottom of the conduction band. The neutral and charged states of V_O always show pos-itive formation energies. Vacancies with charge state 2+ have the highest stability, as has been reported in the literature.