Electronic properties of N-doped and C-doped TiO2: A first-principles study

JUNG YUP LEE, Dept. of Physics, Hanyang University, JAE-WON PARK, Korea Atomic Energy Research Institute, JUN HYUNG CHO, Dept. of Physics, Hanyang University — We present first-principles density-functional calculations for the electronic properties of both a nitrogen-doped and a carbon-doped anatase TiO2 crystal. The 2p states originating from the N and C impurities appear in the band gap of TiO2. The interaction of these states with O 2p states is very weak, resulting in a negligible change of the band gap. This result contrasts with a pervious theoretical analysis where the band gap of the N-doped TiO2 is reduced by mixing N 2p states with O 2p states. Our calculated band structure and charge character of N 2p states are consist with several recent experimental data of N-doped TiO2, which showed that the visible light absorption is due to N 2p states located above the valence band maximum rather than to narrowing of the band gap.