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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.

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