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# Structural and Electronic Properties of $TiO_2$, Nb:$TiO_2$ and Cr:$TiO_2$: A First Principles Study

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Substitutional Nb donor and Cr acceptor states in Anatase and Rutile $TiO_2$ have been studied using generalized gradient approximation (PBE-GGA) employing pseudopotentials and plane wave basis sets in bulk. The calculations reveal that, on doping the Rutile structure with Cr and Nb atoms, new states were found to occur within the band gap, principally between 8.67 eV and 10.56 eV. These states are due to Nb_4d and Cr_3d orbitals. For the anatasse structure, states due to the dopants occurred between 6.663 eV and 8.939 eV. It was also observed that during the 2% doping with Cr and Nb, there were fewer new states in the band gap compared to many new states realized during the 4% doping and this happened in both Rutile and Anatase phases of $TiO_2$. This shows that a higher doping concentration of 4% results in more energy states and hence more carriers, thus making $TiO_2$ a better conductor than either 2% doping or pure $TiO_2$. This study found that doping $TiO_2$ (Anatase and Rutile) with either Cr or Nb at 2% and 4%, resulted in the removal of the energy band gap, implying improved conductivity compared to pure $TiO_2$ [1] which exhibits insulating properties.

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