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AB-INITIO CALCULATION OF THE ELECTRONIC STATES INDUCED BY Nb AND Cr DOPING OF RUTILE AND ANATASE TiO2 .

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In this study, plane wave self consistent field calculations have been performed on the electronic structure of rutile and anatase phases of titanium dioxide (TiO2). To this end ab-initio calculations have been performed for a 48-atom rutile supercell and 96-atom anatase supercell using the plane wave code – Quantum Espresso. Density functional theory (DFT) with hybrid functionals have been used to obtain a more accurate description of the electronic properties of titanium dioxide in addition to the standard exchange-correlation (XC) functionals namely; the local density approximation (LDA) and the generalized gradient approximation (GGA). In this study, the screened hybrid functional of Heyd-Scuseria-Erzehoff (HSE06) has been used. HSE06 is known to overcome most of the shortcomings of both the LDA and GGA XC functionals. Both the titanium dioxide structures were fully optimized by minimizing the local total energy and atomic forces, after which band structure and density of states were calculated. Band gap energies 1.89 eV (rutile), 2.28 eV (anatase) and 2.25 eV (rutile), 2.65 eV (anatase) were obtained using GGA-PBE and HSE06 functionals respectively. Experimental value for band gap is 3.0 eV for rutile and 3.2 eV for anatase. In order to obtain the bulk equilibrium properties, the energy volume curves for the two structures were fitted to the Murnaghan equation of state.
Substitutional chromium and Niobium at the titanium sites was found to introduced new electronic states within the band gap. These new states are discussed with respect to tuning doped titanium dioxide for the application in photocatalysis.

Are you currently a postgraduate student? (Yes/No)

YES

At what level of studies are you currently? (Hons/MSc/PhD)

PhD

Please provide the name and email address of your supervisor.

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