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Electronic and Magnetic Structure of C and N doped rutile-TiO_2: an *ab-initio* DFT study JACQUELINE ATANELOV, CHRISTOPH GRUBER, PETER MOHN, Vienna University of Technology — We study the electronic and magnetic structure of carbon and nitrogen impurities and interstitials in rutile TiO_2. To this end we perform *ab-initio* calculations of a 48-atom supercell employing the VASP code. In order to obtain a realistic description of the size of the band gap, exchange and correlation are treated with functionals beyond ordinary LSDA. Both, atomic positions and cell dimensions are fully relaxed. Substitutional carbon and nitrogen are found to have a magnetic moment of 2 and $1\mu_B$, respectively, with a tendency for anti-ferromagnetic long range order. For C/N on interstitial sites we find that carbon is non-magnetic while nitrogen always possesses a magnetic moment of $1\mu_B$. We find that these interstitial positions are on a saddle point of the total energy. The stable configuration is reached when both carbon and nitrogen form a CO and NO dimer with a bond length close to the double bond for CO and NO. This result is in agreement with earlier experimental investigations detecting such NO entities from XPS measurements. For all configurations investigated both C and N states are found inside the TiO_2 gap. These new electronic states are discussed with respect to tuning doped TiO_2 for the application in photocatalysis.

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