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Incorporation of Non-metal Impurities at the Anatase TiO_2(001)-(1 $\times$ 4) Surface JUN HEE LEE, Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA, DANIEL FERNANDEZ HEVIA, Universidad de Las Palmas de Gran Canaria, Campus de Tafira, 35017 Las Palmas de Gran Canaria, Spain, ANNABELLA SELLONI, Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA — Surface doping of TiO_2 is of special interest because the distribution of impurities at or near the surface can have a significant influence on the photocatalytic properties of TiO_2. We have used first-principles density functional theory (DFT) calculations to determine the incorporation mechanisms of nitrogen (N) and carbon (C), two widely used *p*-type dopants, at the reconstructed (001) surface of anatase, the TiO_2 polymorph most relevant for photocatalysis. Starting from adsorbed impurities, we identify various incorporation pathways and show that the non-exposed oxygen sites just below the surface play a crucial role in accomodating non-metal impurities at the TiO_2(001) surface. Based on the obtained results, we propose strategies which could help to increase the doping concentration and the photocatalytic activity at the TiO_2 surface by exploiting the morphology of the reconstructed surface [1].

[1] Incorporation of Non-metal Impurities at the Anatase TiO_2(001)-(1 $\times$ 4) Surface, arXiv:1209.1602.

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