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Electronic and Optical Properties of Cr-N Co-doped TiO_2 for Intermediate Band Solar Cells KATHERINE INZANI, SVERRE MAGNUS SELBACH, Norwegian Univ Tech (NTNU) — A density functional theory (DFT) study is presented on the effect of Cr and N co-doping on the electronic structure and optical properties of TiO_2. The wide-band gap and high photocatalytic response of anatase TiO_2 place it as candidate host material for intermediate band solar cells. For this application, a suitable dopant and high doping level is required to introduce a mid-gap band, however defect control is still necessary for an efficient photovoltaic device. A proposed solution is non-compensated substitution of two dopants, which can improve the thermodynamic and kinetic solubilities whilst also providing passivation of recombination centers. DFT is used here to predict the effect of non-compensated Cr and N dopant concentrations on the electronic structure of TiO_2, utilizing hybrid exchange correlation functionals to give accurate band gaps. The intermediate band character is further investigated by calculation of absorption spectra. Furthermore, the effect of dopant concentration on anatase and rutile phase stability is evaluated. The results presented are being used to guide experimental studies, advising effective dopant levels and giving structural predictions for material synthesis, and providing optical constants for input to solar cell modelling for cell design.

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