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Effects on the density of states of titanium dioxide by doping with sulfur ARTURO HERNANDEZ ZELEDON, JAMES LEWIS, Department of Physics, West Virginia University — TiO_2 is an attractive material for photocatalytic and photovoltaic applications, even though its maximum absorption happens around 4 eV, and the sunlight irradiance peak is between 1.5eV and 3.1eV. In this work we look for the effects of doping TiO_2 with sulfur, as one way to reduce the gap between the conduction and the valence states. We took the TiO_2 rutile structure as basis for random substitutions, in which we randomly select some oxygen atoms and we replace them with sulfur, making $TiO_{2(1-x)}S_{2x}$ for x = 0.1 and x = 0.25, then we relax the doped structures in order to find the stable configurations, then we select the lower energy structures to carry out the calculation of the density of states as a function of sulfur concentration. All the process and calculations are made using the FIREBALL software.

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