

Abstract Submitted  
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**Effects on the optical properties of titanium dioxide by doping with sulfur** JORGE HERNANDEZ ZELEDON, JAMES LEWIS, West Virginia University —  $TiO_2$  is an attractive material for photocatalytic and photovoltaic applications like water splitting or self cleaning surfaces, but 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, in order to increase the efficiency of Sun light absorption. To modify the optic properties 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  $x = 0.25$ . Here we present our results for the computational calculations of the band gap and absorption as function of concentration. All the process and calculations are made using the FIREBALL software.

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