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UNDERSTANDING THE ELECTRONIC AND OPTICAL PROPERTIES OF TIO2 ANATASE (100) AND (001) SURFACES DOPED AND CO-DOPED WITH SILVER AND CARBON FOR APPLICATION IN DYE-SENSITIZED SOLAR CELL

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Nature of adding some foreign atoms in titanium dioxide (TiO2) play a vital role in increasing its photocatalytic properties. As TiO2 has a large band gap and used in the dye sensitized solar cells, the addition of different elements stabilizes the system and shifts its absorption to the visible spectrum. Density functional theory (DFT) has been used to study a pair of dopants, introduced to understand the electronic and optical properties of Anatase TiO2 (100) and (001) surfaces doped and co-doped with Ag and C. The calculations employ the generalized gradient approximation (GGA). The model surfaces structures were constructed from an optimized Anatase bulk structure. Silver as transitional metals was doped in TiO2 surfaces with one Ti atom replaced by a silver and co-doping was performed with one oxygen atom been replaced by carbon. The results indicate that both doping and co-doping narrows the band gap of TiO2, leading to its improvement in the photo reactivity and simultaneously maintain strong redox potential. The theoretical calculations could provide meaningful guides of developing more activities of anatase TiO2 photocatalyst with visible light response.

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