

Electronic and Optical Properties of Pure and Co-Doped TiO₂

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In this work, we studied the theoretical calculations of electronic and optical properties of pure and co-doped TiO₂. The optical absorption curves of co-doped TiO₂ demonstrate the higher photo-response for visible-light than that of single doped one. The results provided a possible explanation for experimentally optical absorption observed broadening to visible-light in co-doped TiO₂. This could provide theoretical basis for further developing of rutile TiO₂ photo-catalyst and related experimental.

Keywords: TiO₂, theoretical calculations, photo catalyst