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Electronic and Optical Properties of Pure and Co-Doped Tio_2

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In this work, we studied the theoretical calculations of electronic and optical properties of pure and co-doped TiO_2. The optical absorption curves of co-doped TiO_2 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 TiO_2. This could provide theoretical basis for further developing of rutile TiO_2 photo-catalyst and related experimental.

Keywords: TiO_2, theoretical calculations, photo catalyst