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First principle study of Hematite (α-Fe2O3) surface structures doped with Copper (Cu) Titanium (Ti) and Nickel (Ni).

Hematite has attracted research interest for many years due to its application in water splitting. Despite their desirable optical band gap and other attractive features, there are great challenges for the implementation of hematite-based photoelectrochemical cells for water splitting. Doping with transition metals have shown to be a practical solution to overcome some of the limitations faced with hematite to improve its photoelectrochemical (PEC) activity. This study explored two different surfaces of hematite doped with Ti, Cu and Nickel, the surfaces were orientated in the directions (001) and (101). First principle study using the density functional theory (DFT) was adopted for calculations. The results show that the band gap of a bulk structure of hematite is 2.29 eV, doping Ti on surface (101) indicate an improved electric conductivity in the visible light region while, Cu dopant reduces the bang gap by upshifting the valence band maximum to a higher energy level. Previous reports stated that a narrow band is confirmed to result in a low rate of charge recombination by showing a high absorptive coefficient in the visible light region. Nickel on the other hand exhibits an absorptive and conducting surface, with an absorption coefficient of approximately 8.5 x104 cm-1 better than the other doped surfaces. The overall analysis of the result shows an opportunity to a successful photoelectrochemical water splitting.

Apply to be considered for a student ; award (Yes / No)?

YES

Level for award;(Hons, MSc, PhD, N/A)?

MSc

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