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Contribution ID: **96** Type: **Poster (Chemistry SIG)**

First Principles study of Zn/Cu doped hematite surfaces for Photoelectrochemical water splitting

First principles studies of Zn/Cu doped {0001} and {012} surfaces of hematite for enhanced photoelectrochemical water splitting have been carried out. Doping was confined to planes in close proximity to the termination region, precisely from the top most layer to the third inner layer (plane P1, P2 and P3) of Fe atoms. The two surfaces and the three doped layers were found thermodynamically stable. The analysis of electronic properties reveals that even with mono doping of Zn on the top most layer (P1) of the {0001} α-Fe2O3 surface, the band gap can be decreased without impurity states in the band gap which normally acts as recombination centres. Cu doped surface systems do not only decrease in the band gap but also leads to the correct conduction band alignment for spontaneous water splitting. Furthermore, the conduction band minimum (CBM) of P2 and P3 of the {012} surface become wavier and delocalised suggesting improved electron mobility of hematite. Analysis of the charge density difference plots showed concentration of charge mainly at the top of the surface, which is the termination region, which suggests facile transfer of charges to the adsorbed water molecules due to the closeness of the charges to the adsorbate. It is envisaged that surface doping is more beneficial than bulk doping because it reduces the distance moved by the charge carriers and further reduce quick recombination resulting in efficient use of the charges. The concentration of the charges at the surface, the decreased band gap and the absence of recombination centres within the band gap suggest improved photocatalytic activity of the Zn/Cu doped α-Fe2O3 surface.

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Session Classification: Chemistry and Material Science SIG Seminar

Track Classification: Chemistry and Material Science SIG Seminar