Ab Initio Studies of Structure, Electronic and Optical Properties of Sn-doped Hematite

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α-Fe_2O_3(Hematite) has been spotlighted as one of the very promising solar cell materials since it is very stable and environment-friendly. Furthermore, iron is the cheapest and one of the most abundant of all metals in the earth. Even though hematite is capable of absorbing roughly 40% of the solar spectrum, but its practical use has been limited due to the low conductivity, weak optical absorption and rapid carrier recombination. Recently, it has been reported that the substitutional Sn doping significantly increases and improves the solar cell efficiency of hematite. Here, using density functional theory, we study the change in electronic and optical properties of hematite due to the Sn doping, and elucidate the underlying mechanism related to the efficiency increase. We expect that our study can provide key parameters for developing novel hematite-based solar cell device with maximal efficiency.