

Abstract Submitted  
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**Chlorine impurities near stacking fault in CdTe**<sup>1</sup> WALTER ORELLANA, Universidad Andres Bello, EDUARDO MENENDEZ-PROUPIN, Universidad de Chile, MAURICIO FLORES, Pontificia Universidad Catolica de Valparaiso and Universidad San Sebastian — Thin-film cadmium telluride (CdTe) is an important low-cost photovoltaic material. However, transmission electron microscopy has revealed high density of extended defects like stacking faults in as-grown CdTe samples. It has also been observed that the presence of chlorine (Cl) and its interaction with stacking faults plays an important role in the production of high efficiency thin-film CdTe solar cell. Here, we investigate the stability and electronic properties of the Cl impurity at a stacking-fault defect in CdTe, using density functional theory calculations, including hybrid functional. We find that the presence of the stacking fault removes the degeneracy of the valence band maximum, inducing a reduction of the bandgap of about 0.1 eV. When chlorine is incorporated close to the stacking fault, the substitutional Cl<sub>Te</sub> has lower formation energy, showing a *p*-type characteristic. On the other hand, interstitial chlorine (Cl<sub>i</sub>) shows three stable sites with similar formation energies. The most stable one is located at the stacking fault center, exhibiting a half-occupied midgap level.

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