

## First Principles study of Bi doped CdTe thin film solar cells: electronic and optical properties

Y. Seminóvski<sup>a</sup>, P. Palacios<sup>a,b</sup>, P. Wahnón<sup>a</sup>

<sup>a</sup> Instituto de Energía Solar & Dpt. TEAT, ETSI Telecomunicación, Universidad Politécnica de Madrid, Ciudad Universitaria s/n, Madrid, Spain.

<sup>b</sup> Dpt. Física y Química Aplicadas a la Técnica Aeronáutica, Escuela de Ingeniería Aeronáutica y del Espacio, Universidad Politécnica de Madrid, Pza de Cardenal Cisneros, 3, 28040, Madrid, Spain.  
[seminovski@etsit.upm.es](mailto:seminovski@etsit.upm.es)

Nowadays, efficiency improvement of solar cells is one of the most important issues in photovoltaic systems and CdTe is one of the most promising thin film photovoltaic materials we can found. CdTe reported efficiencies in solar energy conversion have been as good as that found in polycrystalline Si thin film cell [1], besides CdTe can be easily produced at industrial scale.

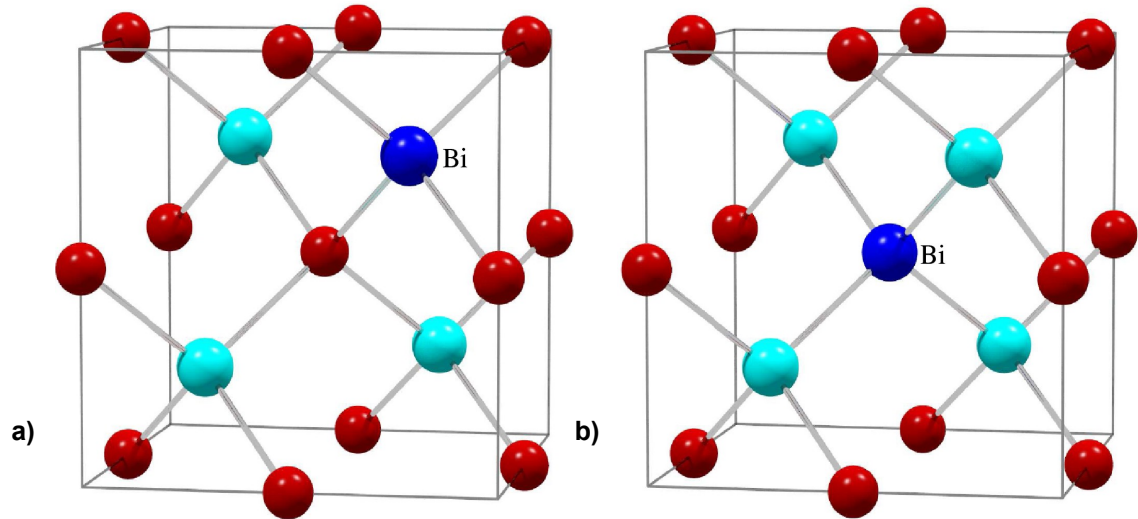
Nevertheless, further higher efficiencies of CdTe can be obtained if some physical properties are enhanced and controlled. Resistivity in CdTe can be controlled by including high concentration of dopant atoms like Bi or Sb inside CdTe crystal. In previous works, experimental results of Bi in concentration over  $1 \cdot 10^{18} \text{ cm}^{-3}$  in CdTe show desirables characteristics as, low resistivity and high photoconductivity [1-3].

In this work, first principles calculations are performed to study the improvement in electronic and optical properties that can be found when Bi is included inside CdTe crystal. Particularly, the electronic-band structures and densities of states of CdTe doped in high proportion with Bi in Cd or Te position, show the formation of states inside the host bandgap. The optical absorption coefficient related with the energy was also obtained and results give higher absorption values for the doped material.

## References

- [1] O. Vigil-Galán et al, Thin Solid Film, **516** (2008) 3818.
- [2] E. Saucedo et al, J. Appl. Phys., **100** (2006) 104901.
- [3] E. Saucedo et al, J. Appl. Phys., **103** (2008) 094901.

## Figures



*CdTe Structure doped with Bi (dark blue) in a) Cd position and b) Te position. Color of Cd (light blue), Te (red).*