Se diffusion and defect passivation role in record performing CdTe photovoltaics

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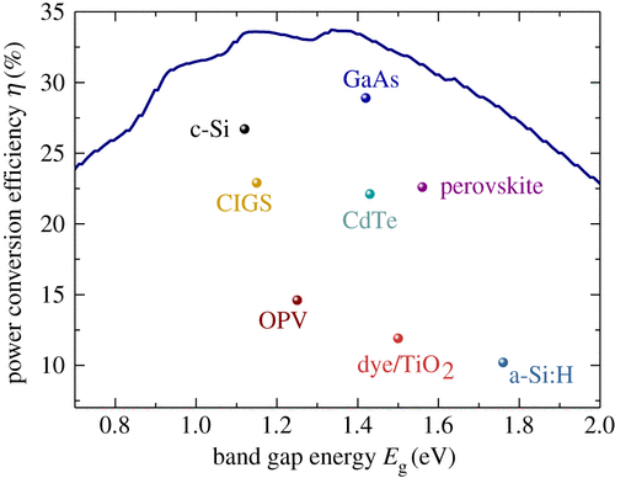
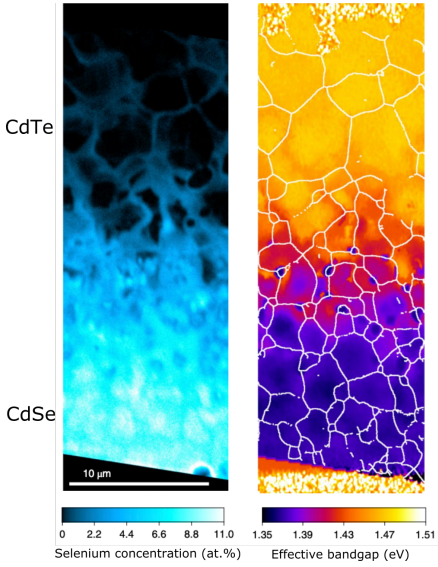
Why CdTe is a effective Solar cell absorber?

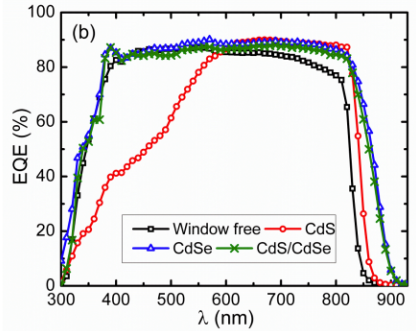


- CdTe has optimal band-gap of 1.46 eV for phtovoltaic application
- Record efficiency of 22.1% achieved by Se alloying of CdTe

*Phil. Trans. R. Soc. A.*377.20180286 *N*

Se alloying impact on CdTe solar efficiency - Macroscopic level



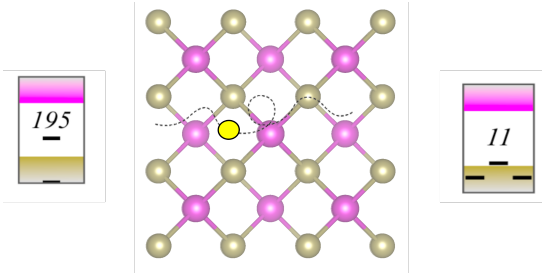


- Fast and long range diffusion of Se in to CdTe leading to band-gap grading.
- In year 2019 it was established that deep (efficiency killer) defect passivation by Se is major reason behind efficiency increase.

Nat Energy 4, 504–511 (2019 *Appl. Phys. Lett.* 105, 183510 (2014)

Microscopic level Se alloying impact on CdTe - unknown

- Microscopic/atomic level mechanism behind Se diffusion and defect passivation by Se atom is still unknown.
- We present/devised out a Density functional theory based simulation account of Se diffusion and defect passivation in CdTe bulk/interior.



Please come to the poster presentation virtual room to discuss our results (Link)

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