

## Supplementary file

### Designing type-II SnSSe/As van der Waals heterostructure with satisfactory oxygen tolerance as an efficient absorber material

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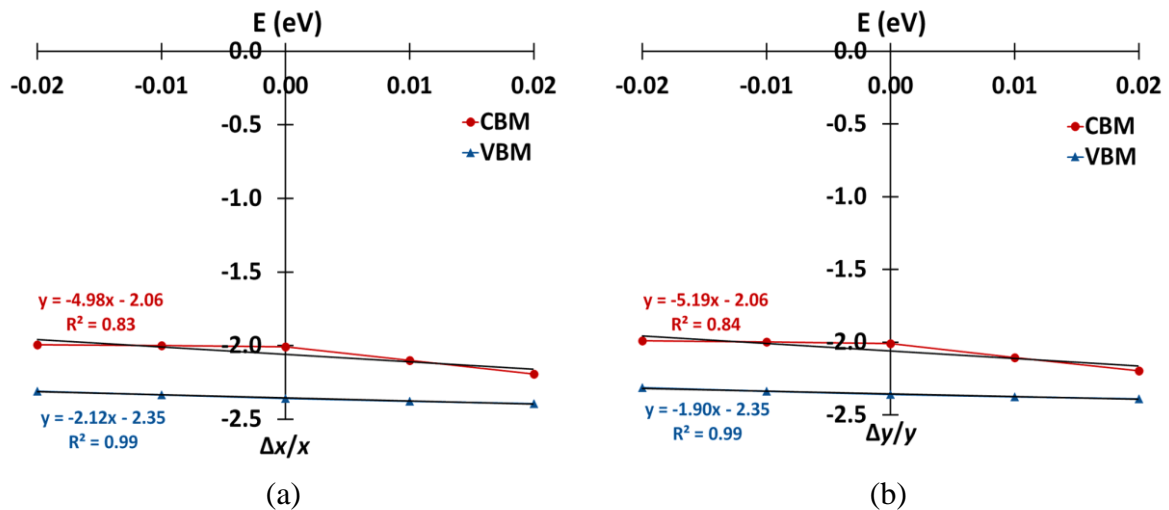
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**S1** Band energies of the CBM and VBM for SnSSe/As heterostructure as a function of lattice dilation along  $x$  and  $y$  directions. The fitted slopes show the  $E_D$  in eV.

## S2 SLME computational details

Theoretical maximum solar cell efficiency can be calculated using the following formula:

$$\eta = \frac{P_m}{P_{in}}$$

where  $P_m$  is the highest achievable power density of the thin-film solar absorber material, while  $P_{in}$  is the incident power density of the entire solar spectrum. The maximum output power density  $P=JV$  of the material can be found utilizing J-V characteristics of solar cell as proposed by Yu and Zunger [1]. Here, J indicates the total current density, while V represents the potential over the absorber layer, as seen in the following relationship:

$$J = J_{sc} - J_r \left( e^{eV/k_B T} - 1 \right)$$

in which  $J_{sc}$ ,  $J_r$ ,  $k_B$  and T denote, respectively, the short-circuit current, the total recombination current density, the Boltzmann constant, and the temperature. Absorptivity  $\alpha(E)$ , photon flux from incident solar spectrum  $I_{sun}(E)$  (AM1.5G) and black-body spectrum  $I_{bb}(E,T)$  can be used to calculate  $J_{sc}$  and  $J_r$ , as follows:

$$J_{sc} = e \int_0^{\infty} \alpha(E) I_{sun}(E) dE$$

$$J_r = e \int_0^{\infty} \alpha(E) I_{bb}(E, T) dE$$

where  $\alpha(E)$  and L are the absorbance coefficient and thickness of the thin film, respectively. Total recombination current density is largely contributed by radiative recombination current density  $J_{rad}$  and non-radiative recombination current density  $J_{non-rad}$ .

[1] L. Yu and A. Zunger (2012). Identification of Potential Photovoltaic Absorbers Based on First-Principles Spectroscopic Screening of Materials. Phys. Rev. Lett. 108, 068701.