

# A Sunlight Cooling Device Based on a 2D van der Waals Heterojunction

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## INTRODUCTION

The quantum yield ( $QY$ ) defines the number of electron-hole pairs generated in a semiconductor (gap  $E_g$ ) by the absorption of a photon of energy  $h\nu$ . In the simplest model we have  $QY=1$  when  $h\nu>E_g$ . However,  $QY>1$  occurs when the excess energy generates extra electron-hole pairs by Coulomb carrier-carrier interaction. This is the impact ionization (II) behaviour [1]. In the ideal case, shown in Fig. 1, a photon of energy  $h\nu>nE_g$  gives  $QY=n$  (with  $n$  a integer). Recent works show that, due to large Coulomb screening, II is particularly strong in few-layers transition metal dichalcogenides (TMD) [2].

In a previous study, we used *ab initio* calculations to compute the electronic band structure of  $\text{MoS}_2/\text{WSe}_2$ , a van der Waals heterojunction based on monolayers of TMD. The absorption coefficient is shown Fig. 2. The gap of this heterojunction is small since  $E_g=0.4$  eV [3]. Here, we show that in contact with a large bandgap reservoir (Fig. 3), under solar radiation and considering an ideal II, it is possible to cool this small gap heterojunction. The sun light generates electron-hole pairs with a large kinetic energy, involving a strong II. The consequence is an accumulation of carriers at the band edges. This excess of carriers can be extracted in a well-designed reservoir by absorbing phonon. We then obtain an evaporative cooling.

## MODEL

To model the carriers in the heterojunction, we assume that their distribution function is a Fermi function at temperature  $T_c$  with a difference between the Fermi levels of electrons and holes given by  $\Delta\mu=\mu_c-\mu_v$ , where  $\mu_c$  ( $\mu_v$ ) is the Fermi level of electrons (holes) in the conduction (valence) band. To calculate  $T_c$  and  $\Delta\mu$ , we consider a detailed balance model:

$$\begin{cases} J_{gen} = J_{rec} + J_{contact} \\ P_{gen} = P_{rec} + P_{contact} + P_{phonon} \end{cases}$$

We present the different terms of this equations in Fig. 4.  $J_{gen}$  is the carrier flux generated by the sun light, considering the absorption of the heterojunction (Fig. 2) and an ideal II.  $J_{rec}$  is the

recombination flux, considering both radiative and non-radiative recombinations.  $J_{contact}$  is the flux of carriers between the heterojunction and the reservoir.  $P_{gen}$ ,  $P_{rec}$  and  $P_{contact}$  are respectively the power flux-densities corresponding to the fluxes  $J_{gen}$ ,  $J_{rec}$  and  $J_{contact}$ .  $P_{phonon}$  is the exchanged power between the carriers and the phonons and is assumed proportional to the difference of carrier and phonon temperatures [4]. When the carrier temperature  $T_c<300$  K, the carriers absorb phonons and  $P_{phonon}<0$ . If this heat absorption is greater than the heat emitted by the non-radiative recombination, the heterojunction is cooled. We define the cooling efficiency as:

$$\eta_{cooling} = \frac{-P_{phonon} - P_{rec,non\ rad}}{P_{gen}}$$

## RESULTS

Fig. 5 shows the temperature  $T_c$  as a function of  $E_{cv}$ , the gap of the reservoir. We get  $T_c<300$  K ( $P_{phonon}<0$ ) if both  $E_{cv}<0.98$  eV and the II is considered. The detailed balance equation shows that  $P_{phonon}$  is more negative as  $P_{contact}$  is larger.  $P_{contact}$  is proportional to the flux of extracted carriers, multiplied by the extraction energy. The II increases the number of carriers and the energy increases with  $E_{cv}$ . Nevertheless, if  $E_{cv}$  is too high, the flux is reduced. The best trade-off is obtained for  $E_{cv}=0.85$  eV. As shown Fig. 6, where  $\eta_{cooling}$  is represented versus  $E_{cv}$ , this corresponds to a maximum efficiency of 61%.

## CONCLUSION

We propose a cooling device which uses the sun as the only source of energy. This concept could have practical applications in nanoscale cooling.

## REFERENCES

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- [4] M. Giteau et. al., *Identification of surface and volume hotcarrier thermalization mechanisms in ultrathin GaAs layers*, JAP, **128**, (2020)

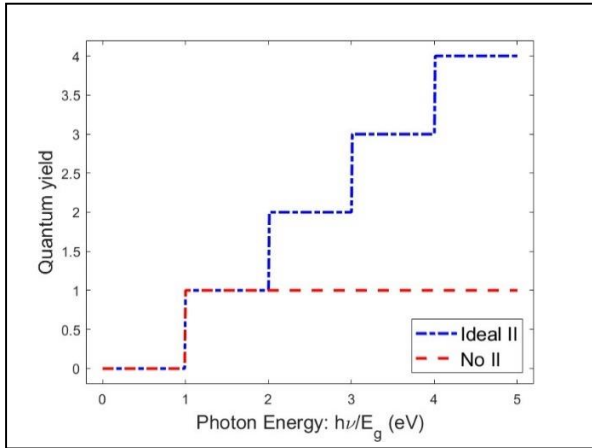


Fig. 1. The quantum yield (QY) is shown as a function of  $h\nu/E_g$  where  $h\nu$  is the photon energy and  $E_g$  is the gap of the semiconductor. The blue curve shows the QY under ideal impact ionisation (II) and the red curve shows the QY without II.

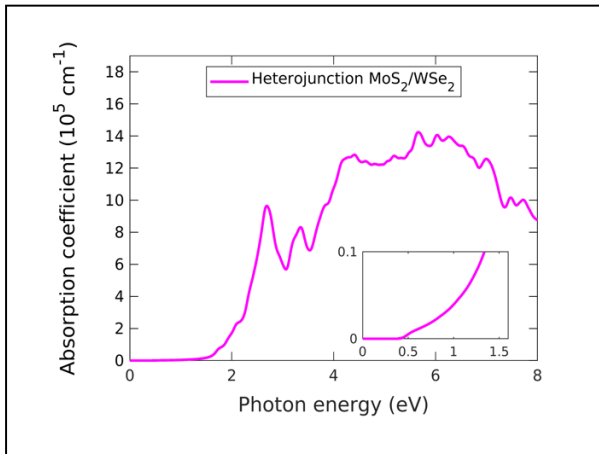


Fig. 2. Absorption coefficient of the MoS<sub>2</sub>/WSe<sub>2</sub> heterojunction, computed with DFT calculation. The inset plot is a zoom in the low energy range.

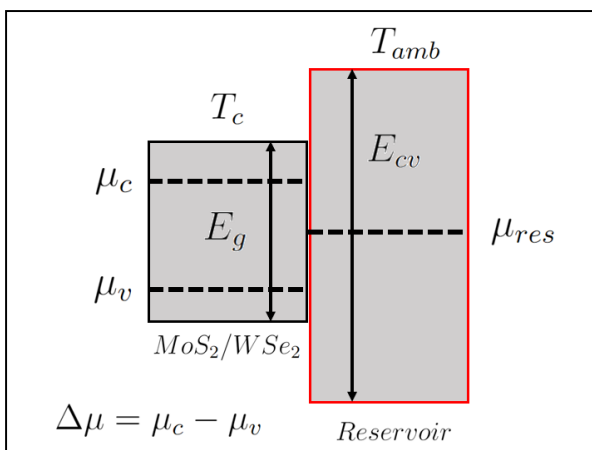


Fig. 3. Band diagram of our device where the MoS<sub>2</sub>/WSe<sub>2</sub> heterojunction (bandgap  $E_g = 0.4$  eV) is in contact with a reservoir (bandgap  $E_{cv} \geq E_g$ ).  $\mu_c$  ( $\mu_v$ ) is the Fermi level of electrons (holes) in the conduction (valence) band.  $\mu_{res}$  is the Fermi level in the reservoir.  $T_c$  is the carrier temperature in the heterojunction.  $T_{amb} = 300$  K is the ambient temperature.

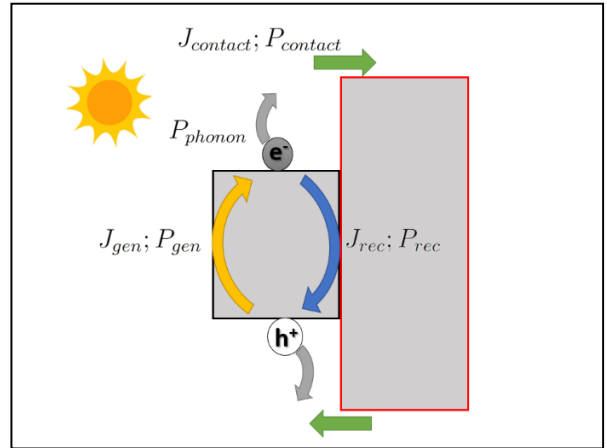


Fig. 4. Carriers fluxes and power flux densities displayed on the band diagram of the device. We consider an isolated system. Thus, carrier exchanges occur only between the small gap heterojunction and the reservoir.

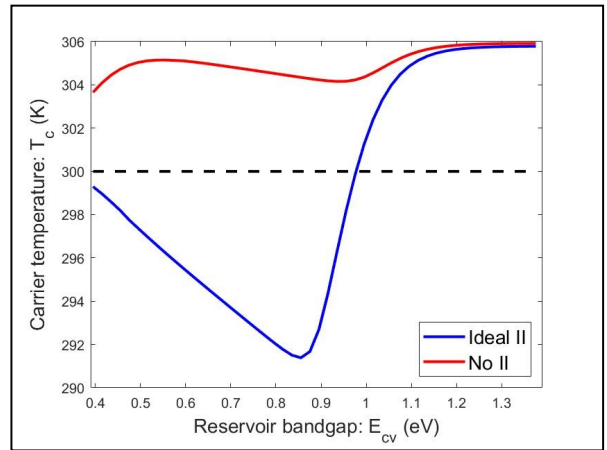


Fig. 5. The carrier temperature  $T_c$  is shown with ideal (blue curve) and without (red curve) II, as a function of the reservoir bandgap  $E_{cv}$ . The black dashed line stands for  $T_c = 300$  K.

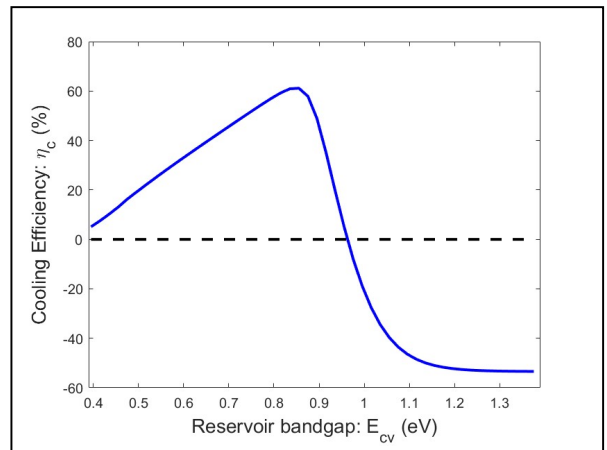


Fig. 6. The cooling efficiency  $\eta_{cooling}$  is shown with ideal II as a function of the reservoir bandgap  $E_{cv}$ . The black dashed line stands for  $\eta_c = 0$  %.