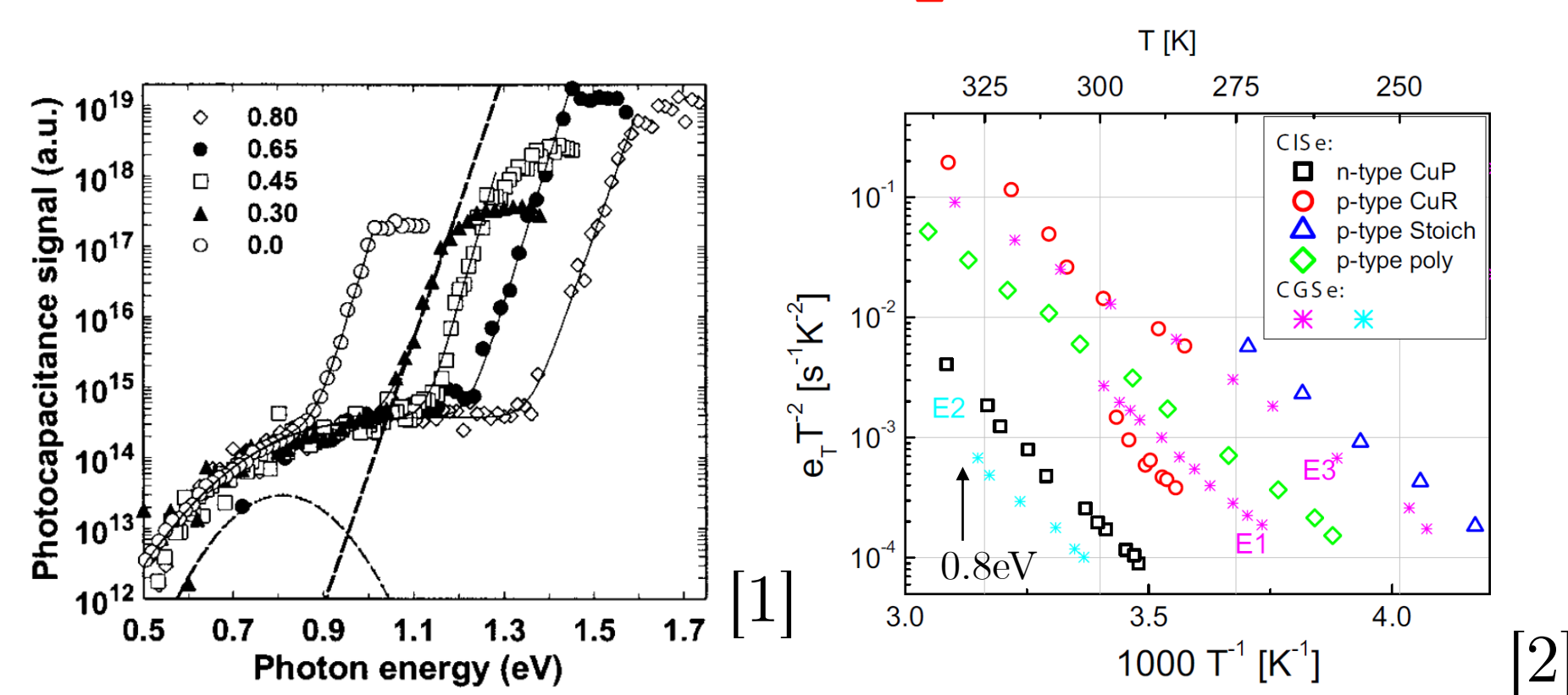


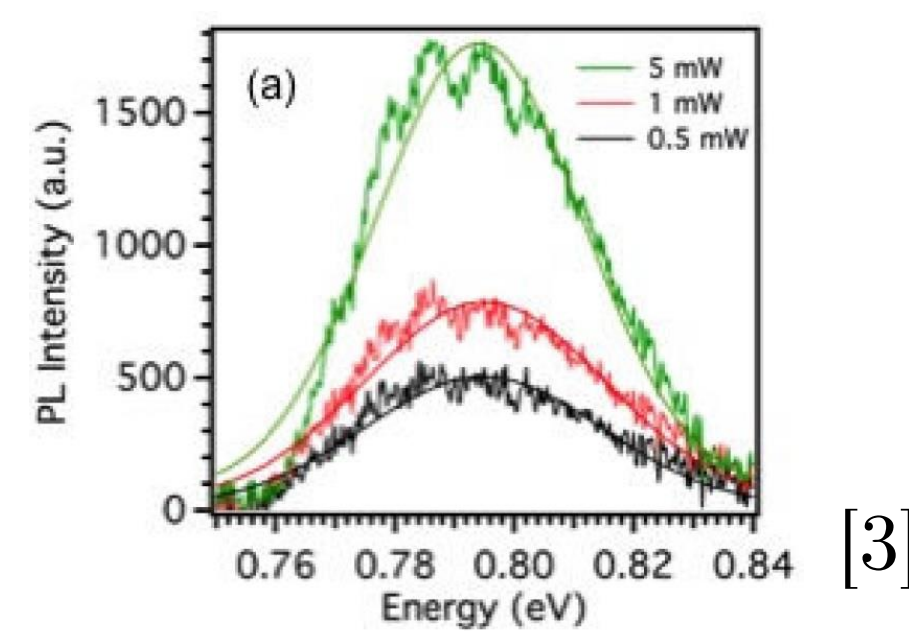
## Motivation

- photocapacitance measurements reveal defect signature at 800 meV above valence band [1]
- signal appears independent of Ga/(Ga+In) ratio and in ternary compounds  $\text{CuInSe}_2/\text{CuGaSe}_2$
- if the signal is caused by defects, we should observe the levels in photoluminescence measurements
- by extending our setup we perform defect spectroscopy on thin films down to 400 meV

## Literature: Experiment



- defect just observed in experiments with excitation



- 0.8 eV defect observed by photocapacitance [1]
- independent of Ga/(Ga+In) ratio in  $\text{Cu}(\text{In},\text{Ga})\text{Se}_2$
- PICTS shows defect response around 0.8 eV in epitaxial/polycrystalline  $\text{CuInSe}_2$  and  $\text{CuGaSe}_2$  [2]
- recently PL transition shown at 0.8 eV [3]

## Experimental details

- samples grown by MOVPE on SI-(100)-GaAs

	$\text{CuInSe}_2$	$\text{CuIn}_{0.7}\text{Ga}_{0.3}\text{Se}_2$	$\text{CuIn}_{0.5}\text{Ga}_{0.5}\text{Se}_2$	$\text{CuIn}_{0.2}\text{Ga}_{0.8}\text{Se}_2$	$\text{CuGaSe}_2$
GGI	0	0.27	0.46	0.8	1
CGI	1.25	0.99	1.29	1.13	1.18

- InAs-detector, range down to 0.4 eV (3100nm)
- InGaAs-array, range down to 0.77 eV (1610nm)

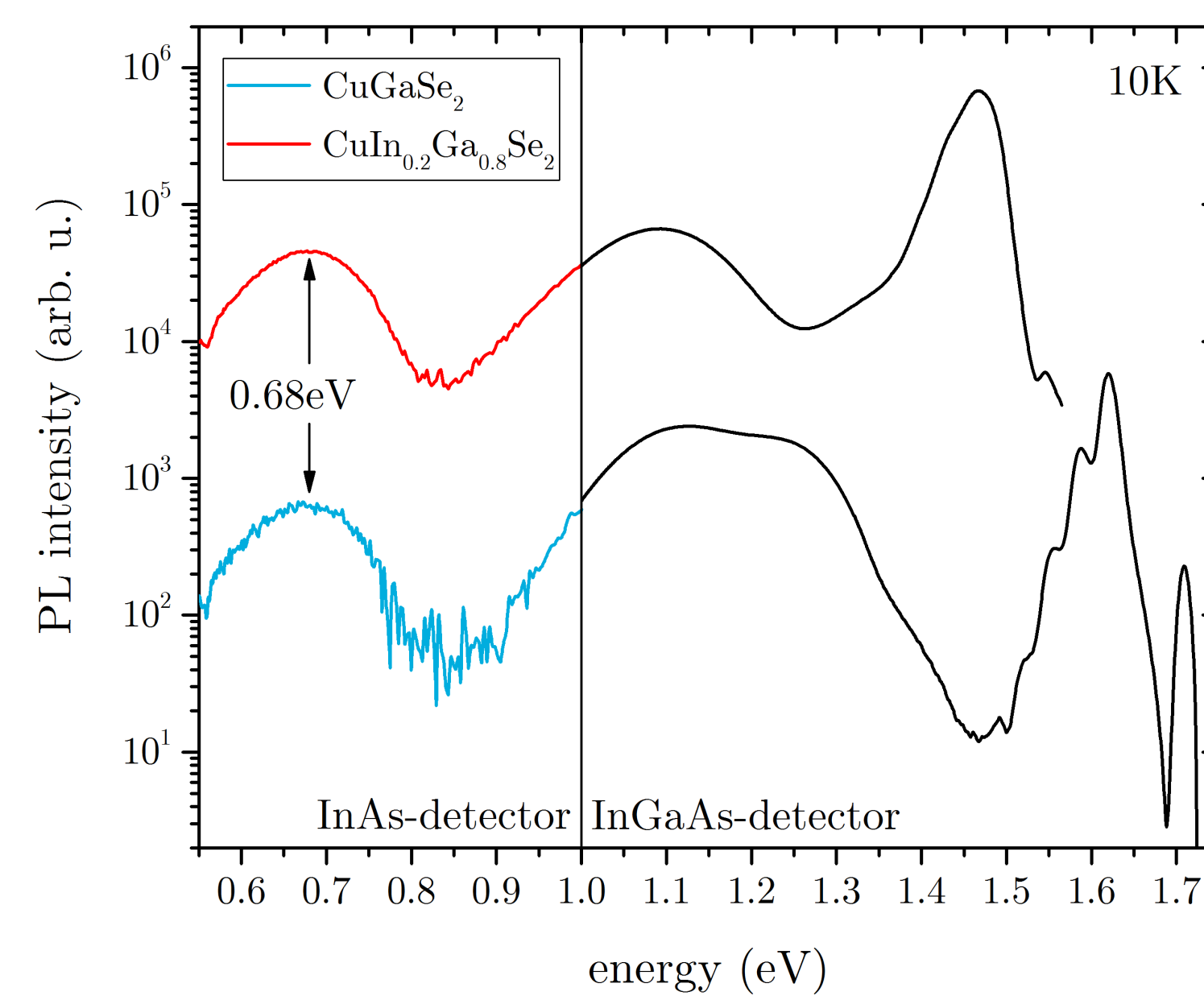
## Acknowledgements

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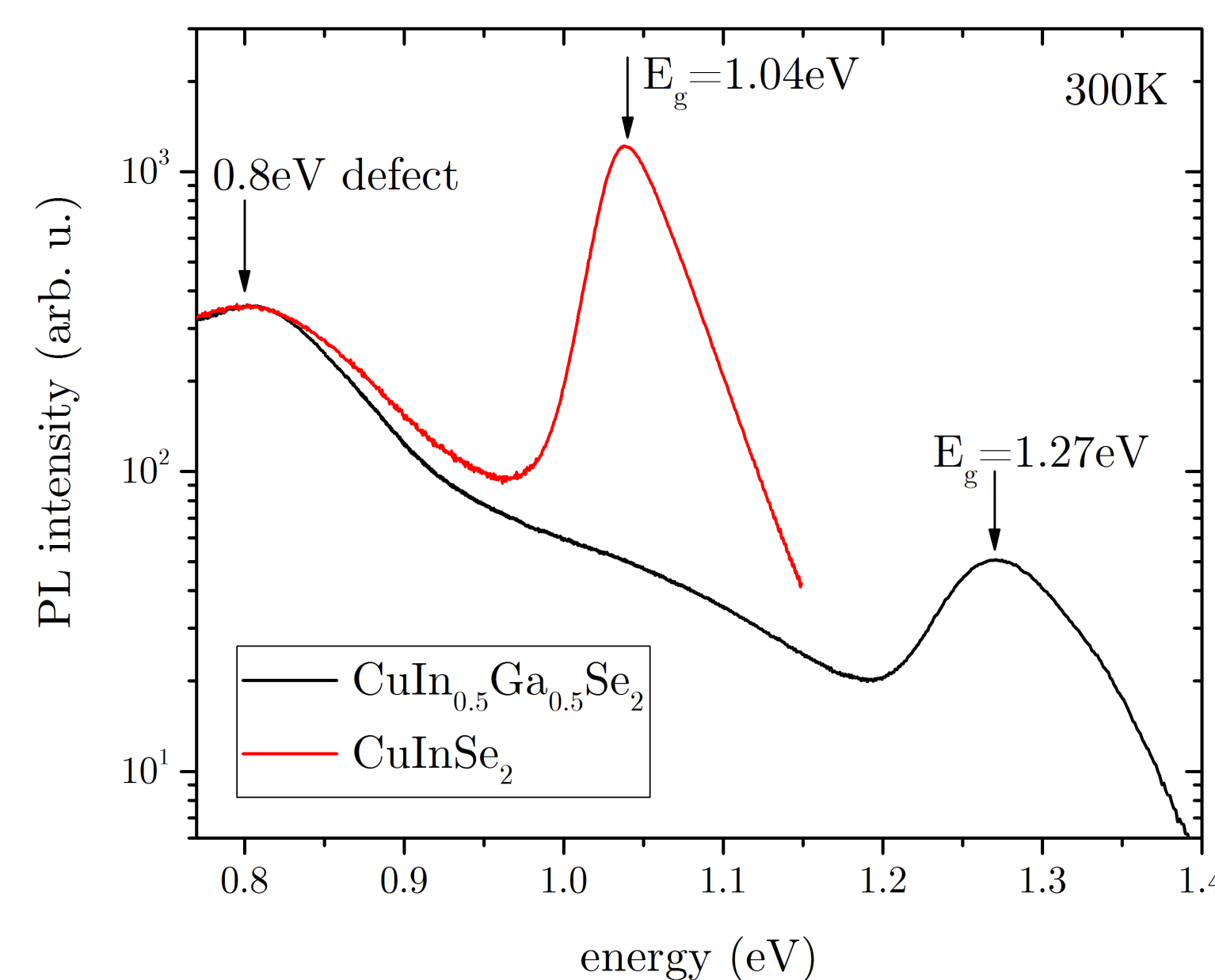
- [1] Heath et. al., Appl. Phys. Lett. 80 (24), 2002  
 [2] Krysztopa et. al., J. Phys. D: Appl. Phys. 45 (335101), 2012  
 [3] Mansfield et. Al., IEEE 42nd PVSC, 2015  
 [4] Yee et. al., Phys. Rev. B 92 (195201), 2015  
 [5] Malitckaya et. al., Adv. Electron. Mater. 1600353, 2017  
 [6] Pohl et. al., Phys. Rev. B 87 (245203), 2013

## Photoluminescence 10K



- transition at 0.68 eV most likely DA-transition into dominant shallow acceptor at 100 meV
  - deep level remains constant when adding Indium
- ⇒ defect level exists around 0.7 - 0.8 eV

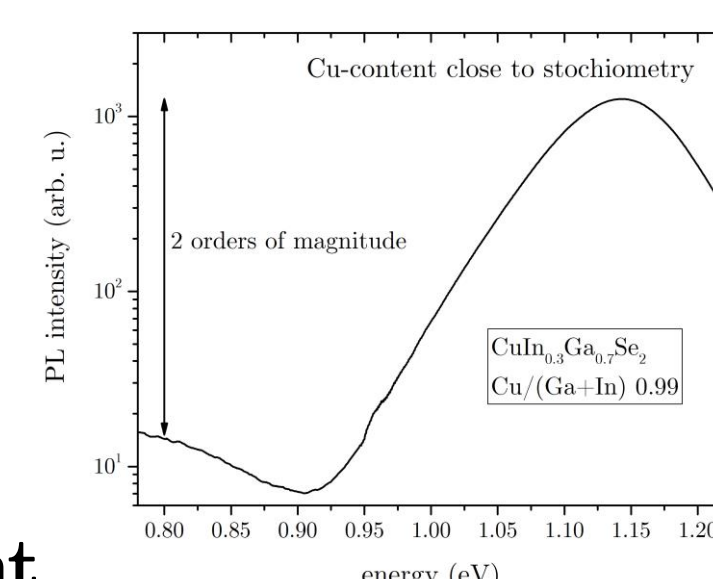
## Deep defect observable at 300K?



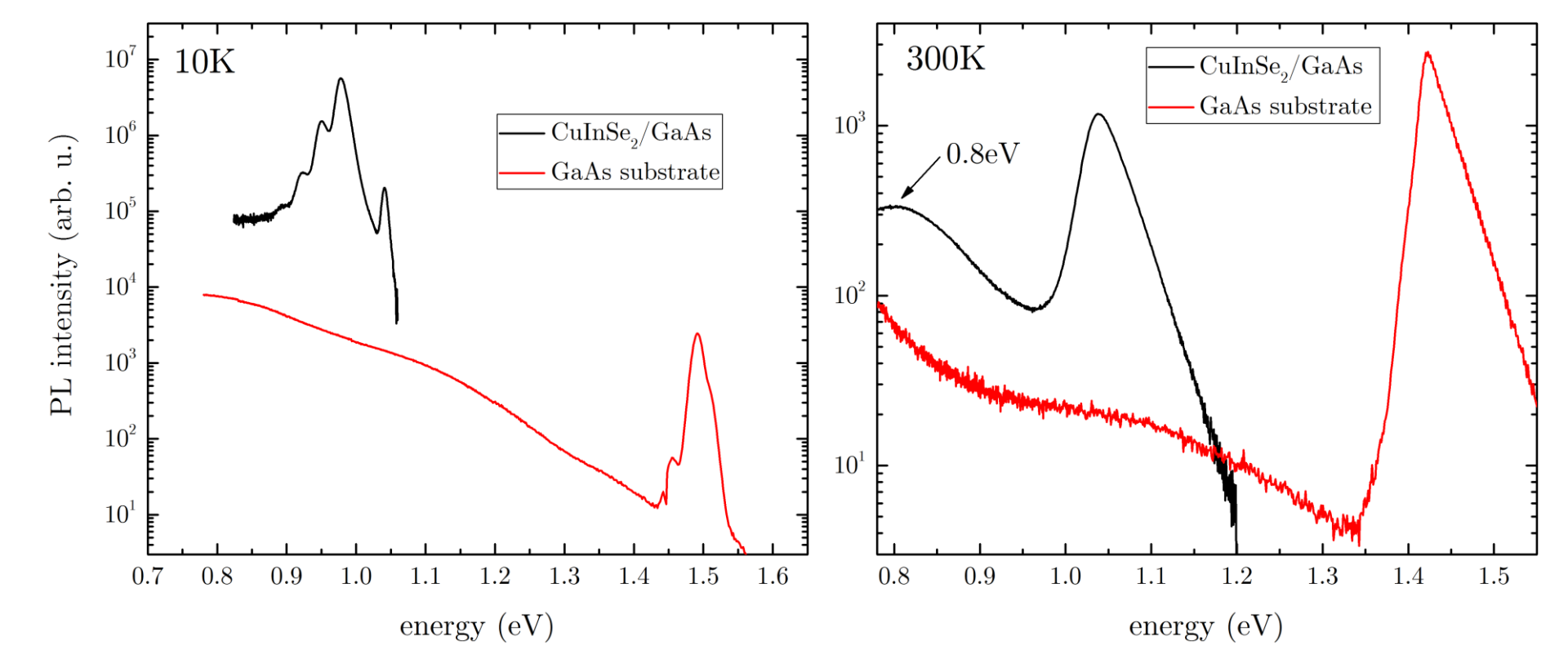
- defect transition at 0.8 eV for room temperature
- **free-to-bound transition** ⇒ defect level at 0.8 eV
- observed in Cu-rich  $\text{CuInSe}_2$  and  $\text{Cu}(\text{InGa})\text{Se}_2$

## What about lower Cu-contents?

- 0.8 eV defect peak not observed in state-of-the-art absorber with GGI approx. 0.3 and CGI approx. 0.9
- Sample B with CGI 0.99 shows smallest defect signal
- **0.8 eV signal decreases with respect to band-band transition for lower Cu-content**

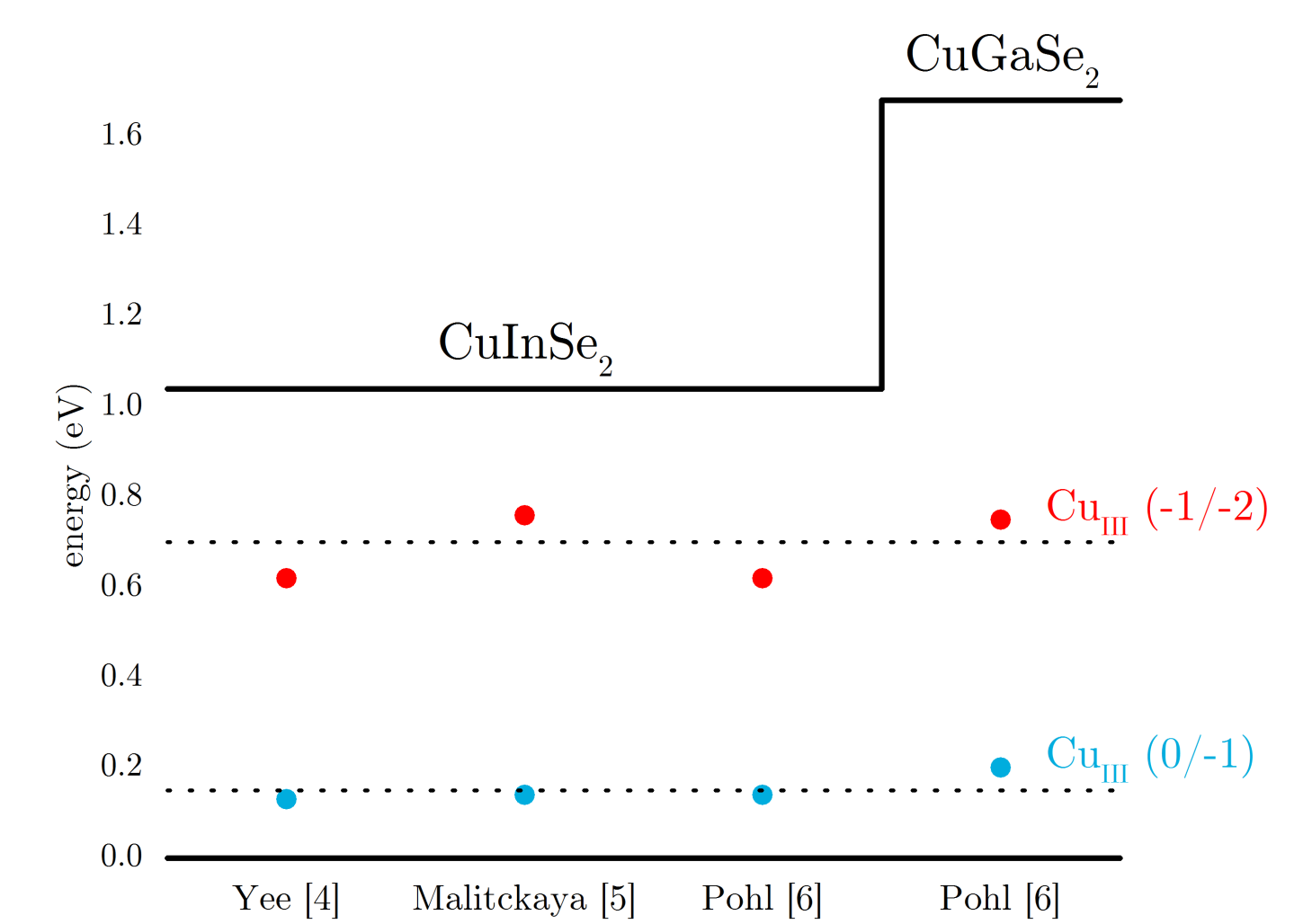


## GaAs-substrate luminescence?



- GaAs has known EL2 defect ( $\text{As}_{\text{Ga}}$  antisite) with optical transitions around 0.7 eV
  - PL signals with direct substrate-illumination have lower intensities than for  $\text{CuInSe}_2/\text{GaAs}$
- ⇒ deep defect transitions not correlated to substrate

## Literature: Theory



- calculations predict the charge transition  $\text{Cu}_{\text{III}}(-1/-2)$  at 0.6 - 0.8 eV above the VBM in  $\text{CuInSe}_2$
- Pohl et. al. calculated  $\text{Cu}_{\text{Ga}}(-1/-2)$  at the same level
- under most preparation conditions  $E_f$  close to VB:  
⇒ no direct formation of  $\text{Cu}_{\text{III}}^{-1}$   
⇒ **photoexcitation needed to charge  $\text{Cu}_{\text{III}}^{-1}$**

## Conclusion

- transition at 0.7 eV for 10K, at 0.8 eV for 300K
- deep defect level remains constant for varying GGI
- defect level not observed in Cu-poor compositions
- defect level attributed to  $\text{Cu}_{\text{III}}(-1/-2)$  antisite
- possible reason for loss of  $V_{\text{OC}}$  in Cu-rich solar cells