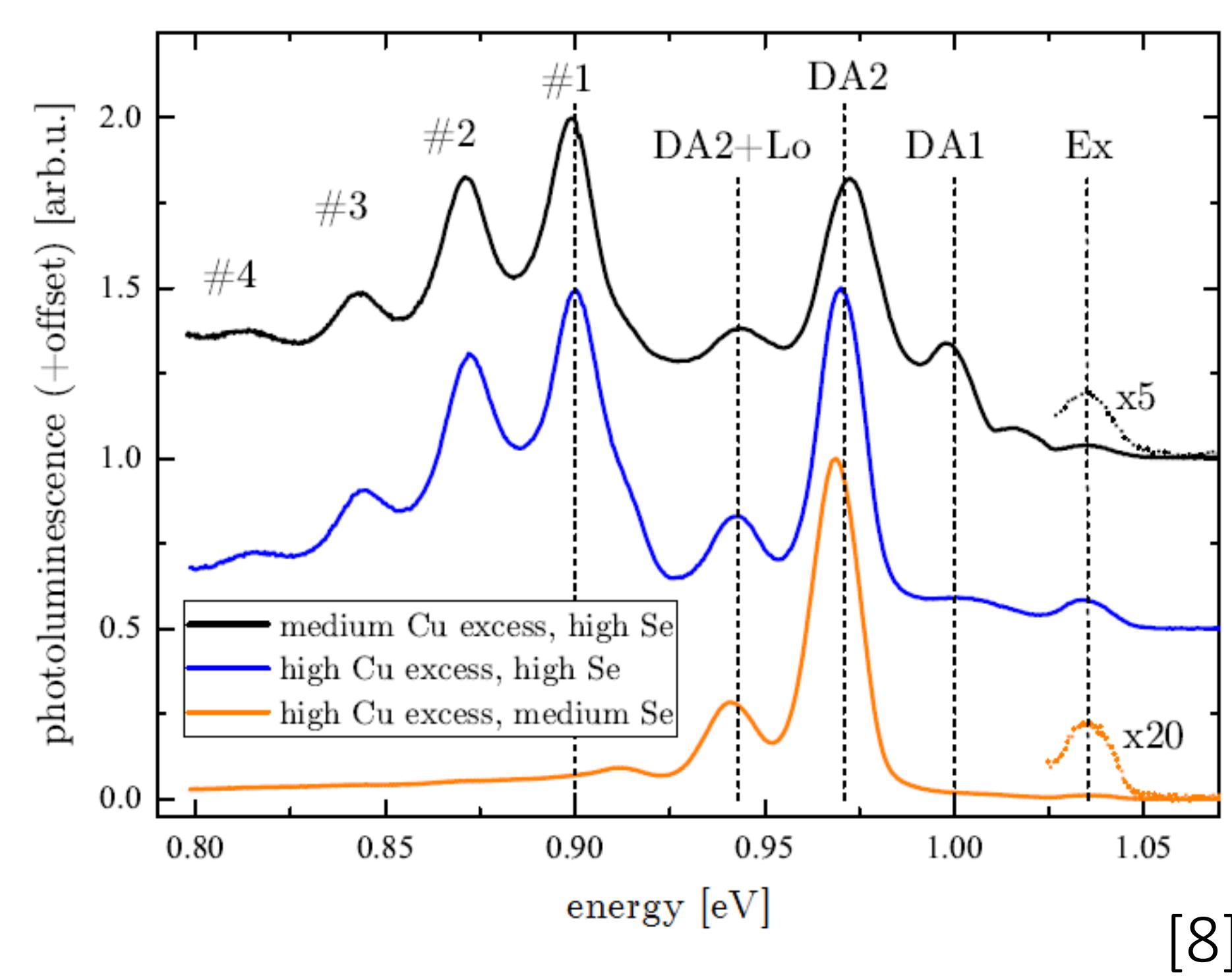
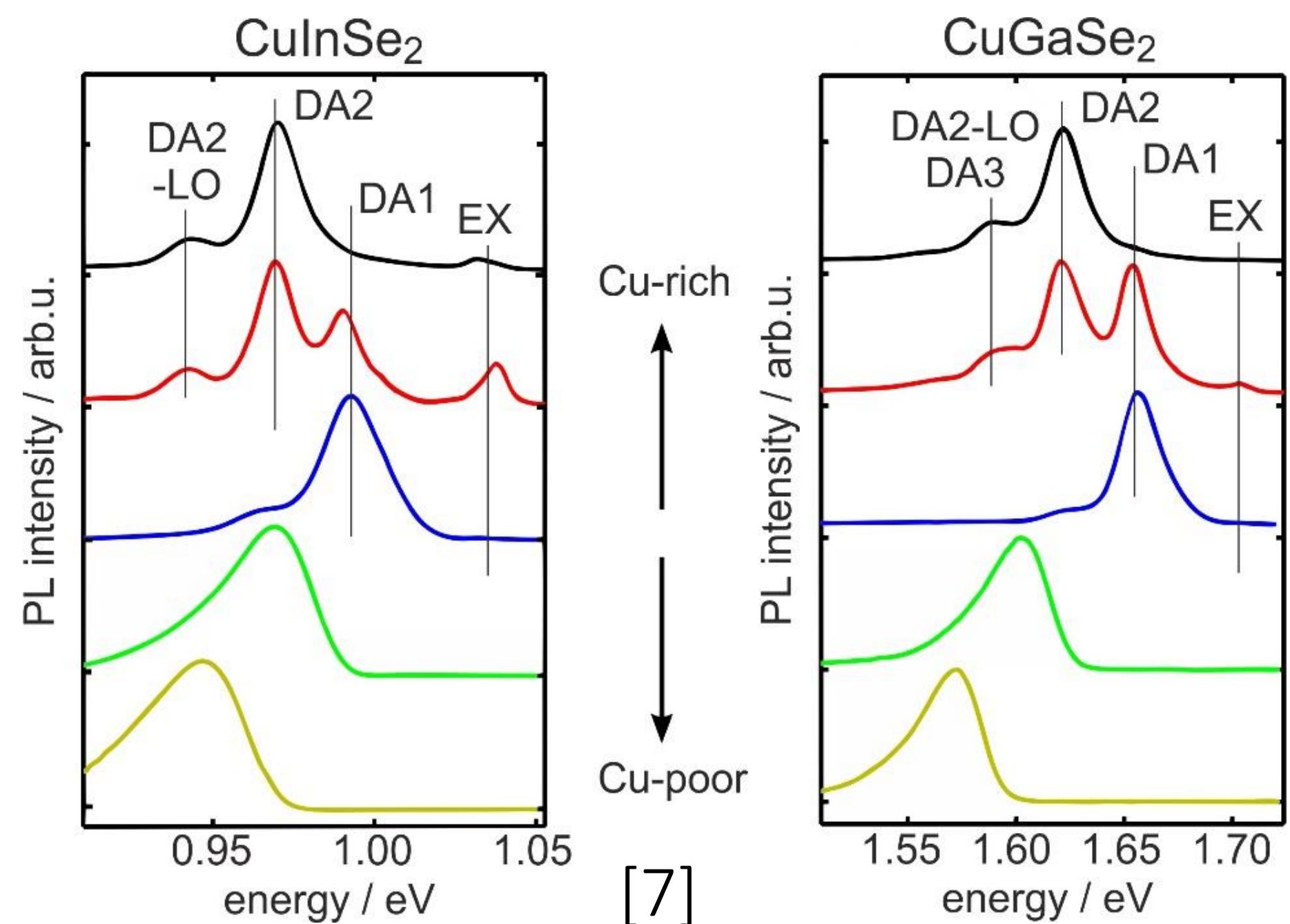
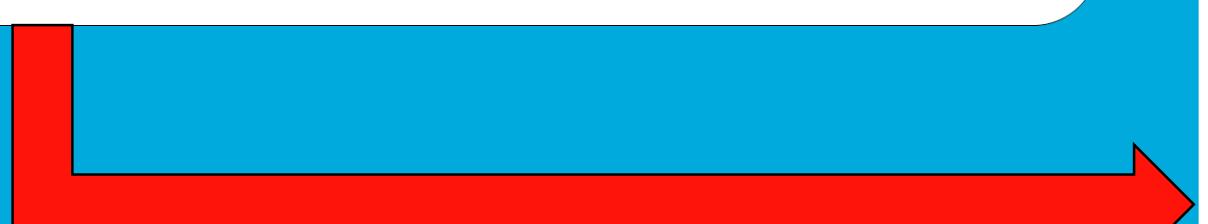


Shallow defects

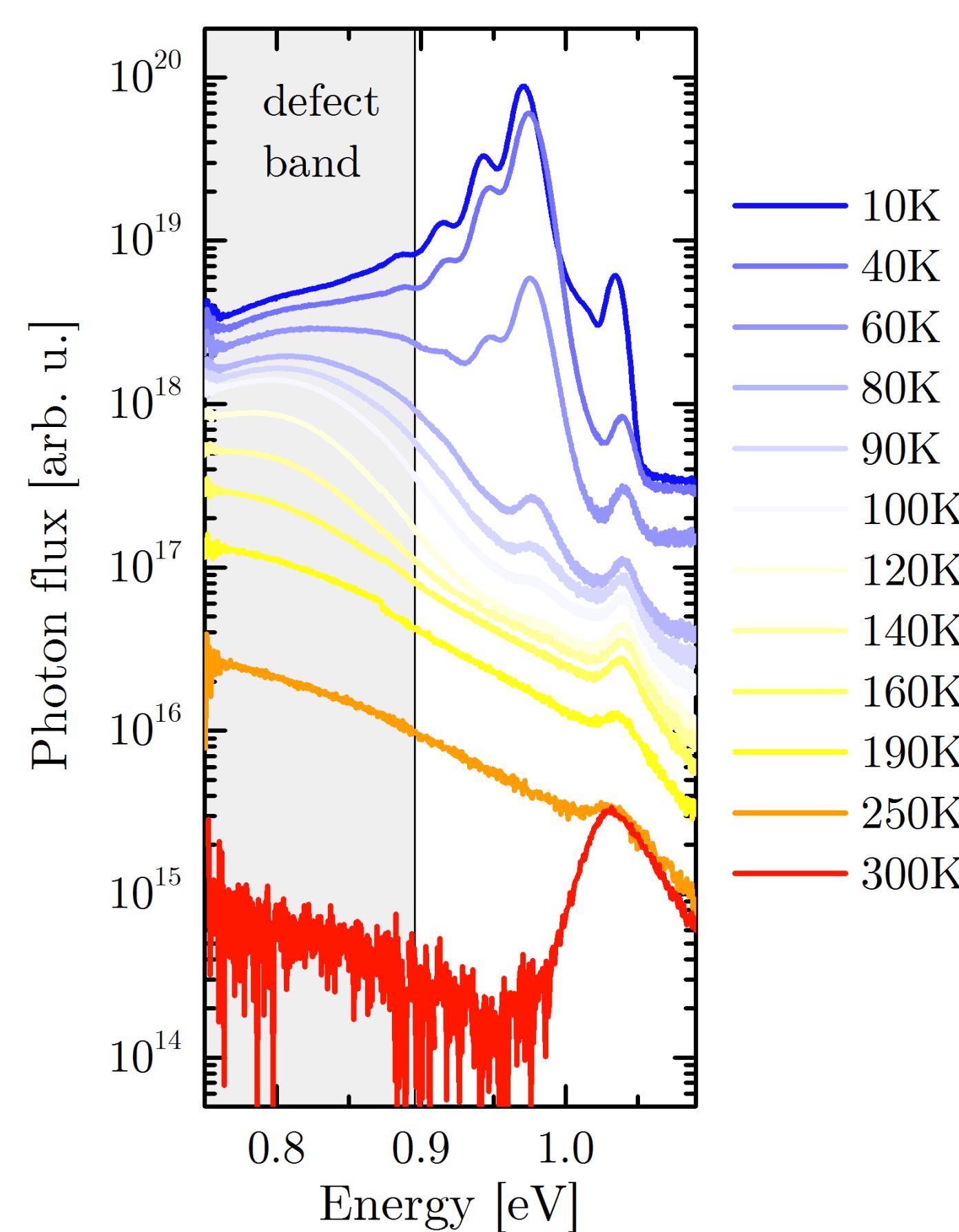
- low temperature photoluminescence (10K)



- D1: shallow donors **8-14 meV** (ClSe/CGSe)
- A1: stoichiometric low-Cu (**40/60 meV**)
- A2: stoichiometric high-Cu (**60/100 meV**)
- A3: CuInSe₂ with high selenium (**135 meV**)
 CuGaSe₂ close to Cu/Ga = 1 (**135 meV**)

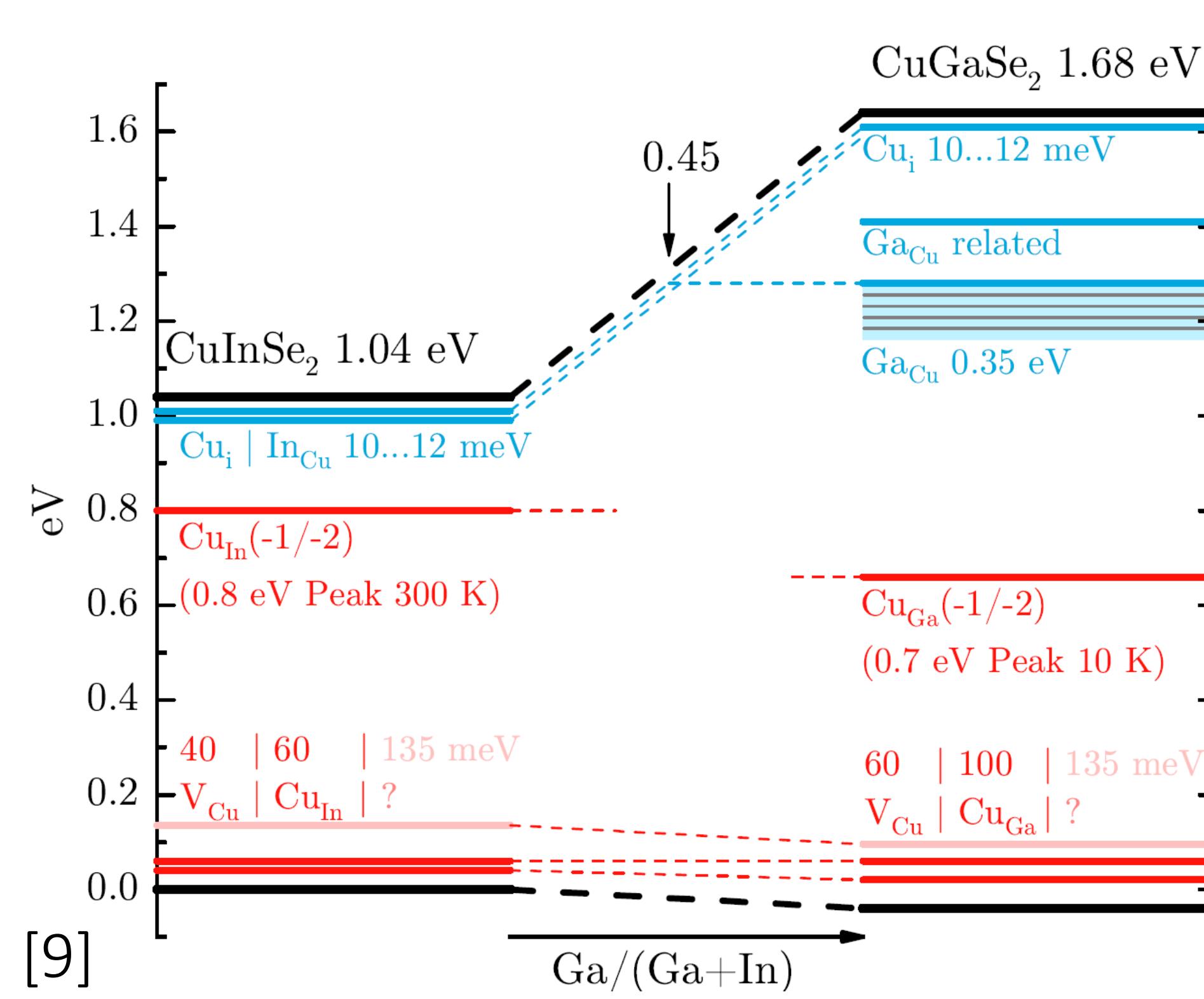


Deep 0.8 eV defect



- 0.8 eV above valence band for varying GGI
- Broad density of states (ca. 0.1 eV)
- Always observed in Cu-rich compositions

Defect model in Cu(In,Ga)Se₂



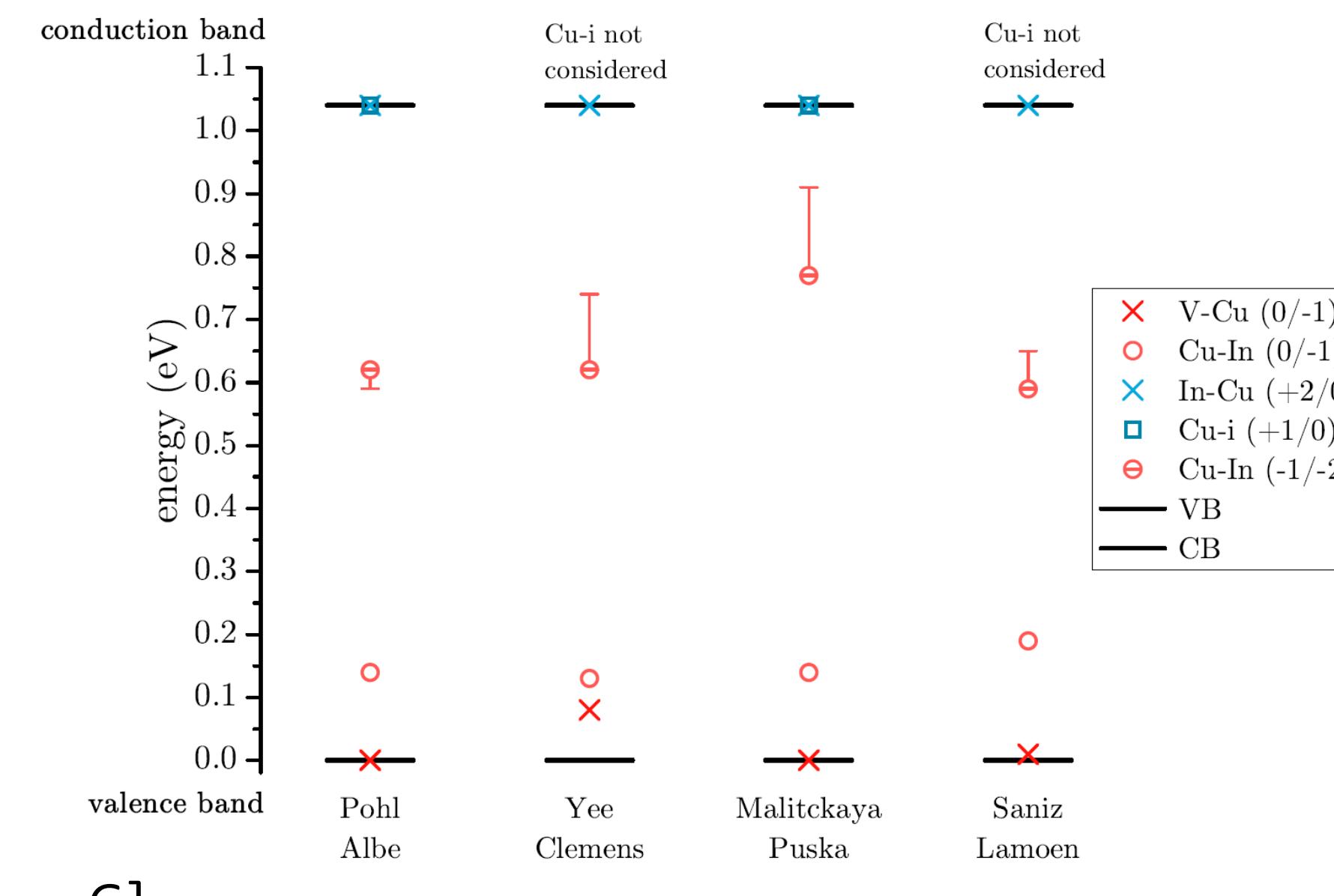
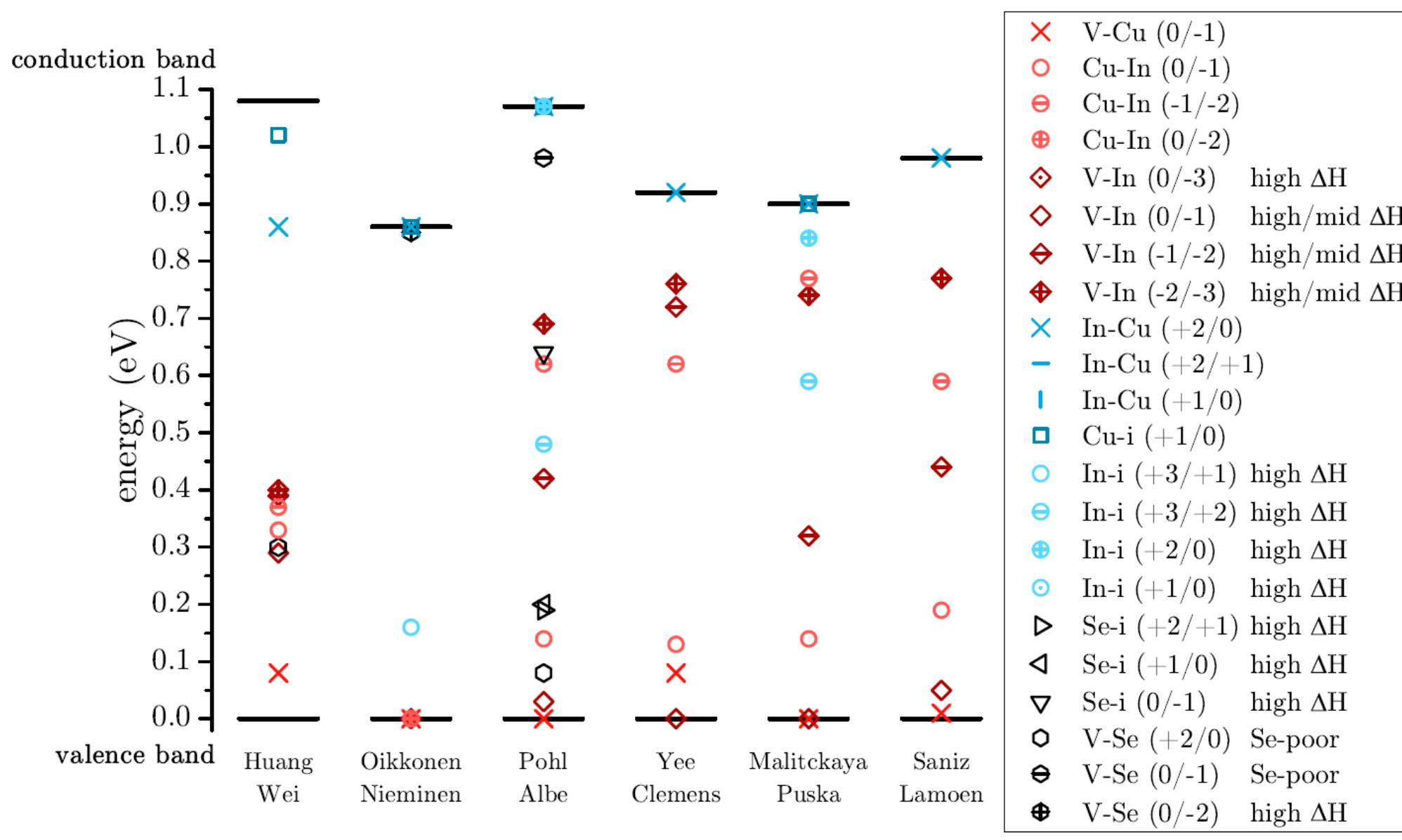
Defects from Theory

Strong agreement for CuInSe₂:

- In_{Cu} and Cu_i shallow donors (D1)
- V_{Cu} shallowest abundant acceptor (A1)
- Cu_{In} fairly shallow, abundant acceptor (A2)
- Cu_{In}(-1/-2) deep charge transition

Few calculations for CuGaSe₂:

- Similar levels with indium/gallium exchange
- But difference: In_{Cu} shallow in CuInSe₂
 Ga_{Cu} deep in CuGaSe₂
- Several Ga_{Cu} levels 1.16 – 1.33 eV above VBM



Literature

[1] Huang/Wei, JPV 4, 2014
 [2] Oikkonen/Nieminen, JPH 26, 2014
 [3] Pohl/Albe, PRB 87, 2013

[4-6]

[4] Yee/Clemens, PRB 92, 2015
 [5] Malitckaya/Puska, AEM, 2017
 [6] Saniz/Lamoen, PCCP 22, 2017

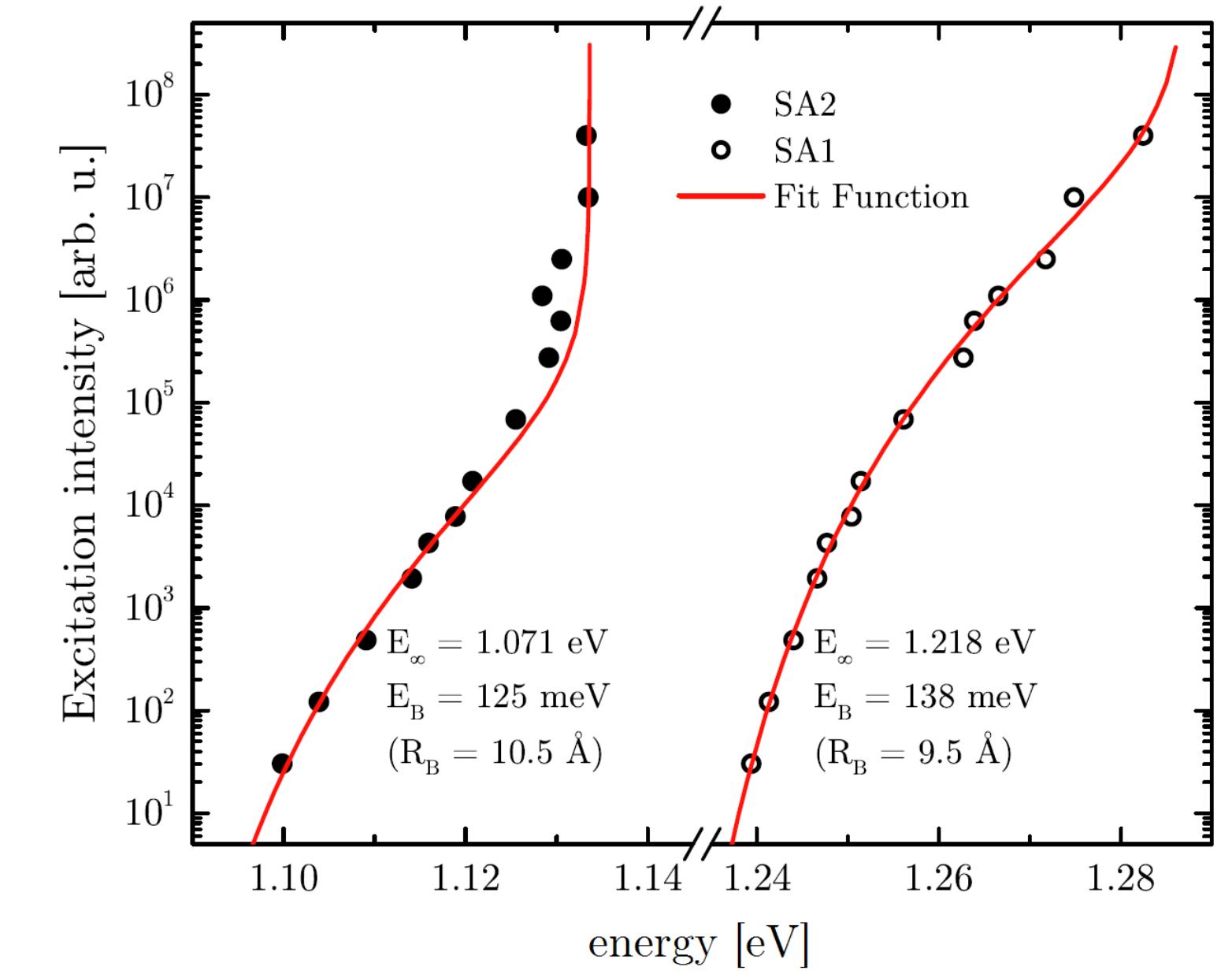
[1-6]

[7-9]

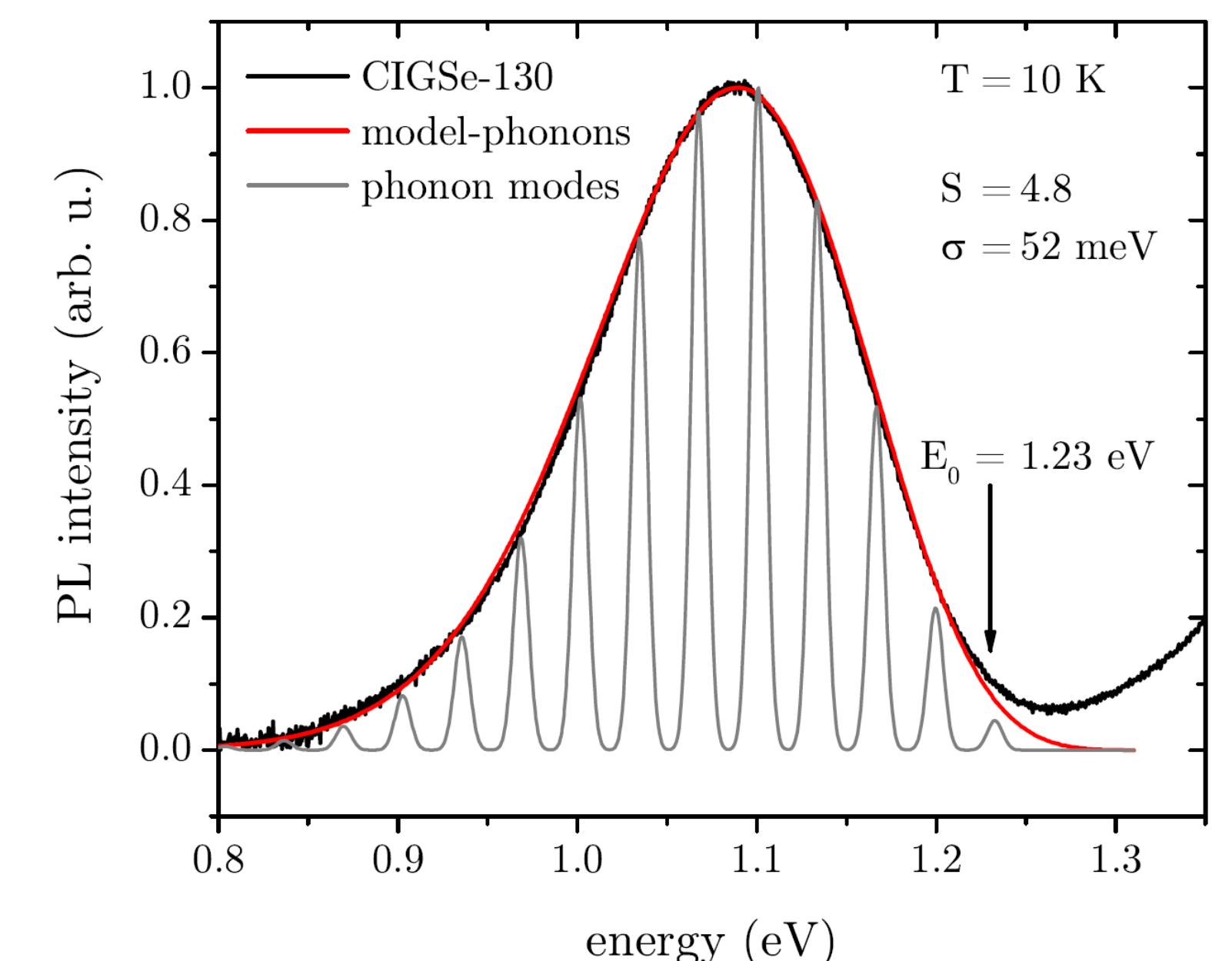
[7] Siebentritt et. al., SEMSS 119, 2013
 [8] Babbe/Siebentritt, under review
 [9] Spindler, PhD Thesis, 2018

Deep 1.3 eV defect

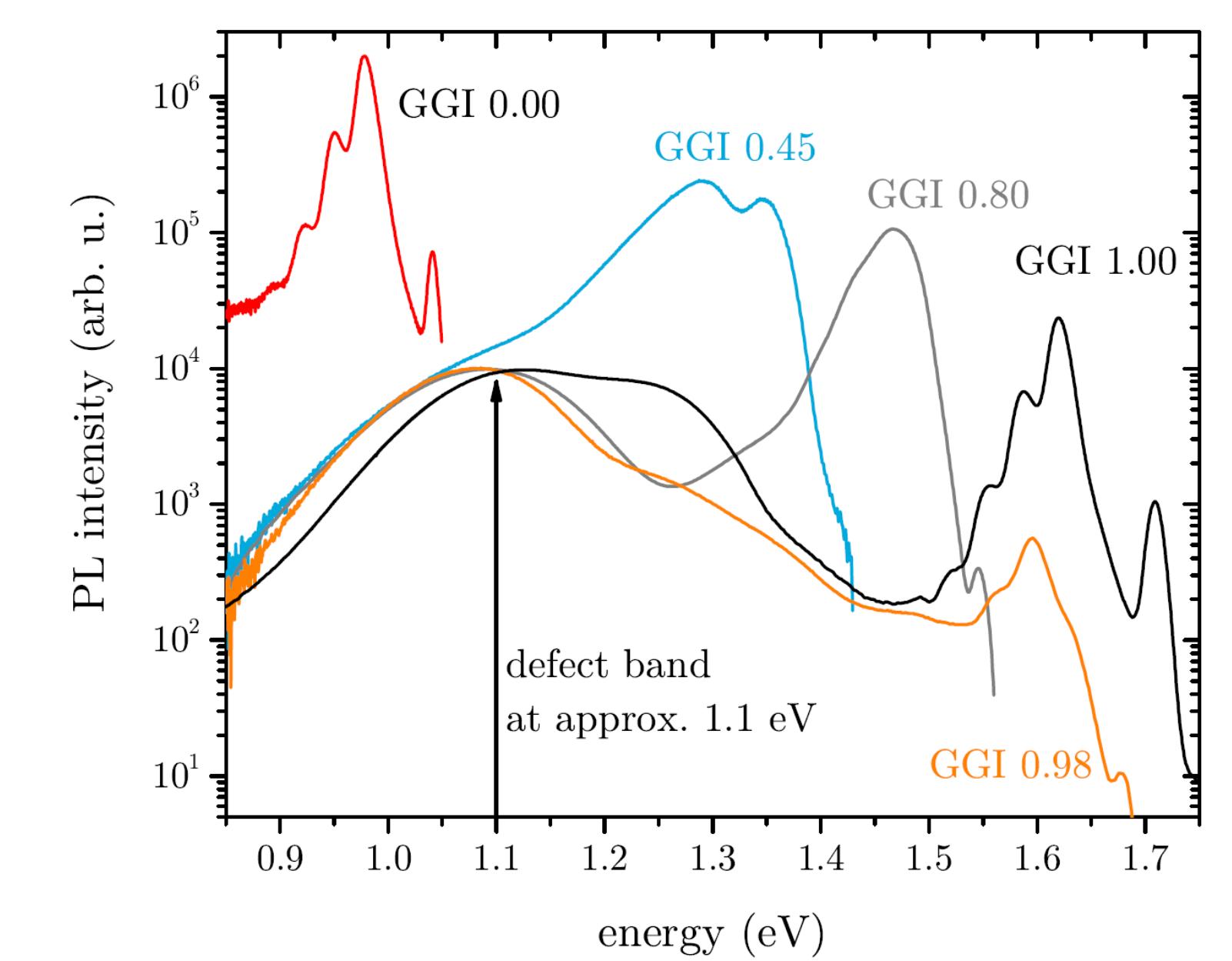
- Large blueshift of 2 deep bands in CuGaSe₂
 → Donor-acceptor pairs with shallow accept.



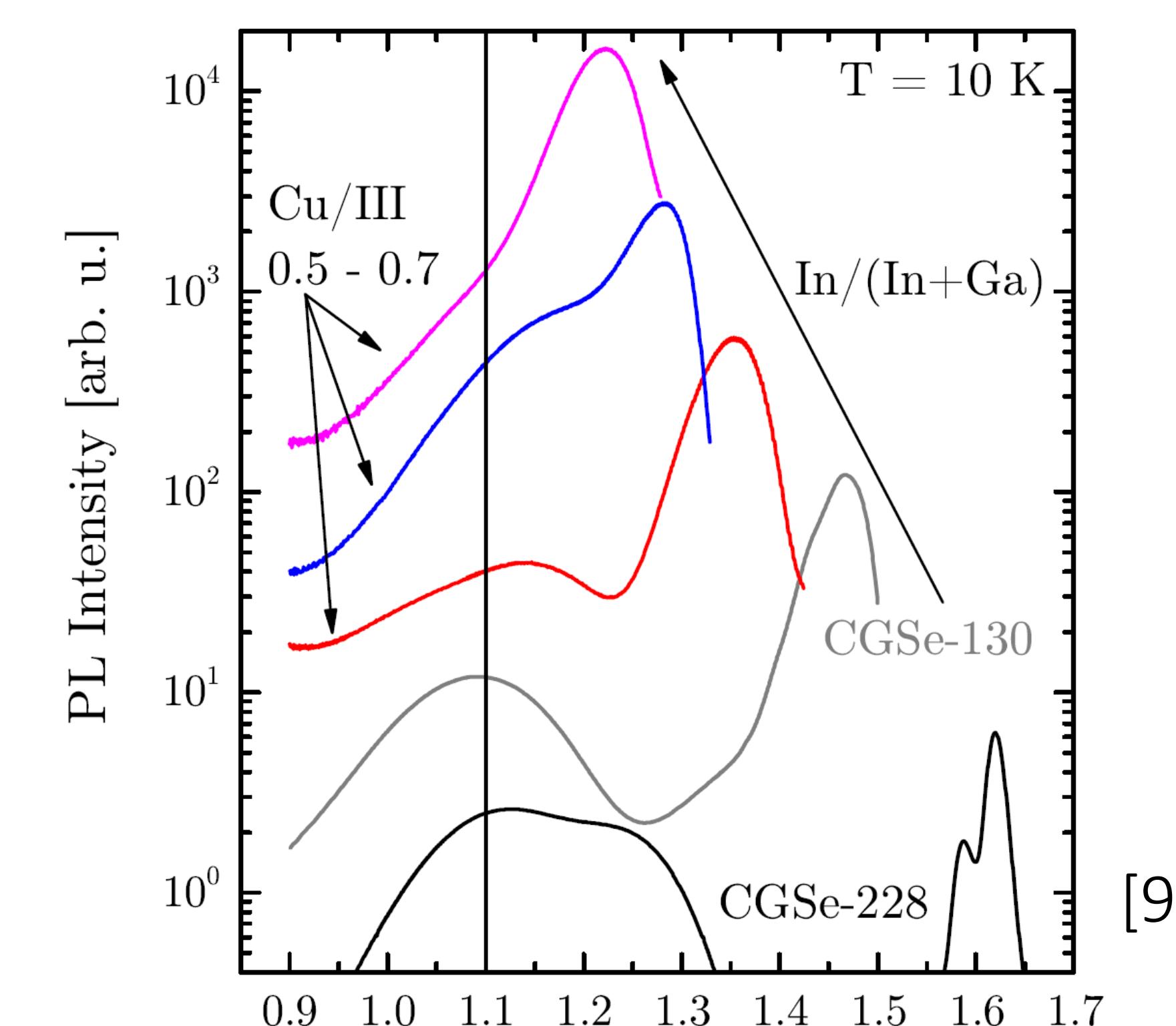
- With 20% of indium: single deep band
 → Determination zero-phonon line 1.23 eV
 → Deep donor-like defect around 1.3 eV



- 1.3 eV above valence band for varying GGI
- Phonon coupling (Huang-Rhys factor ≈ 5)
- GGI < 0.45 Shallow defect
- GGI > 0.45 Recombination center



- Also observed in Cu-poor compositions



Acknowledgements

Florian Werner, Max Wolter