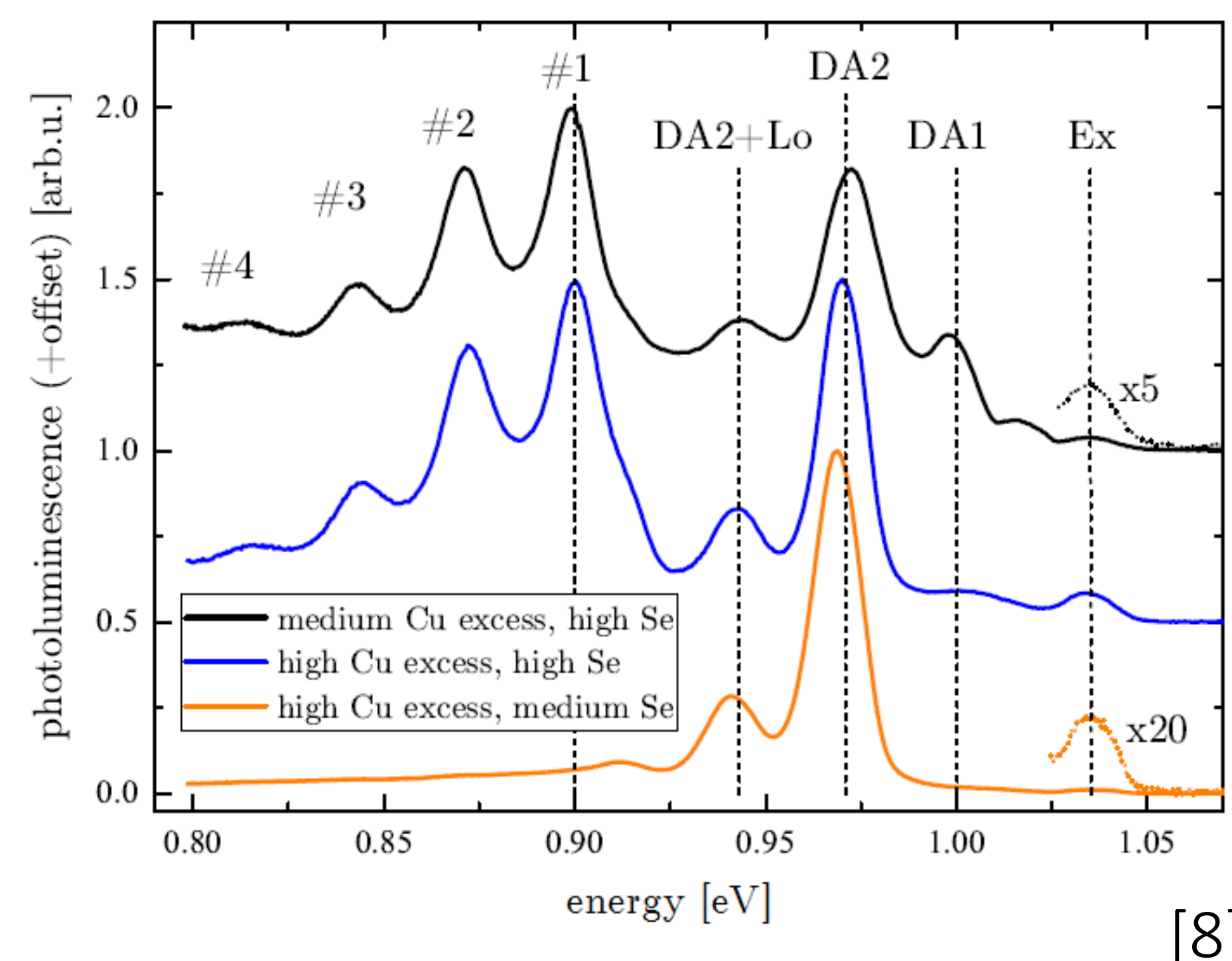
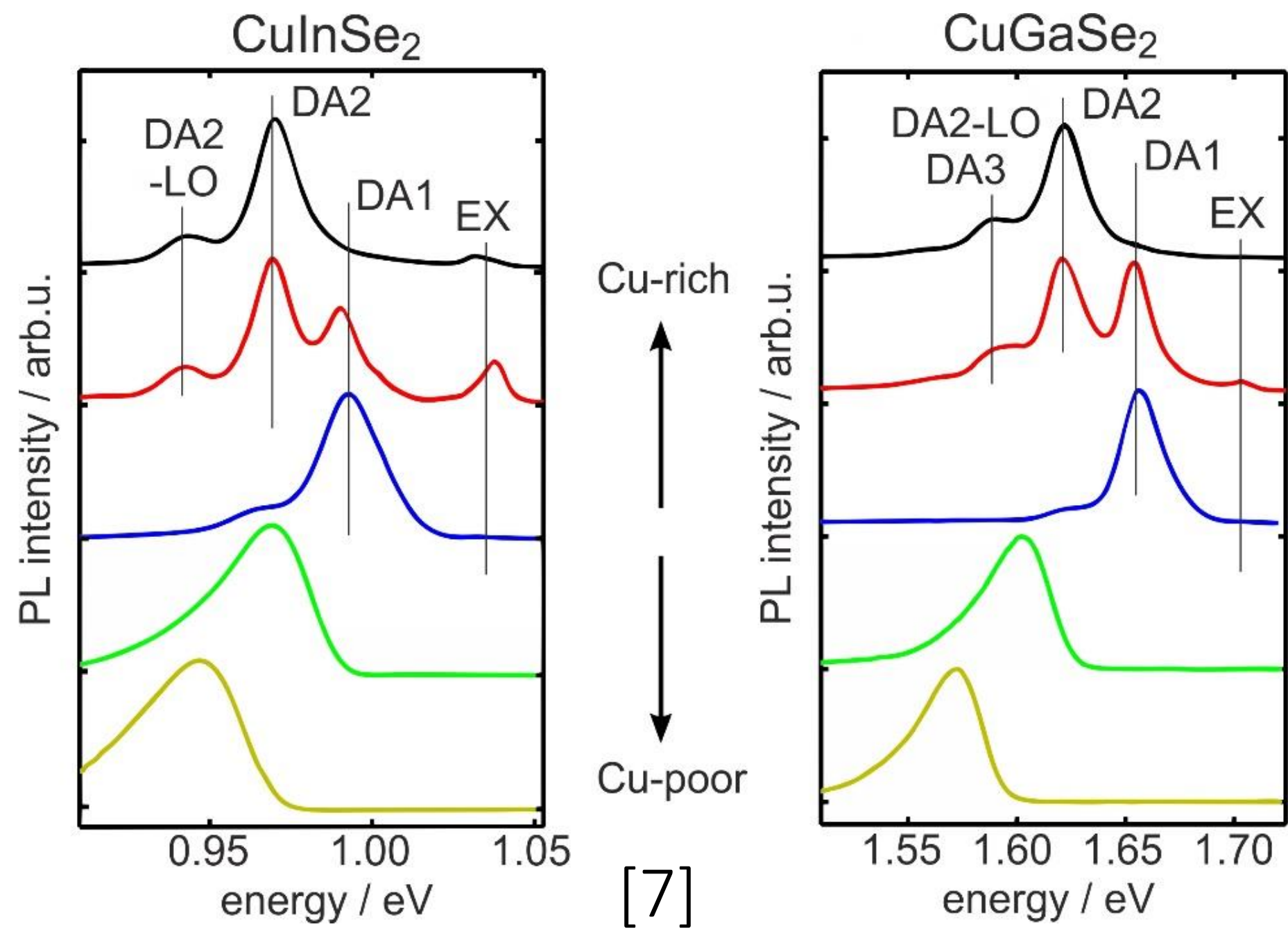


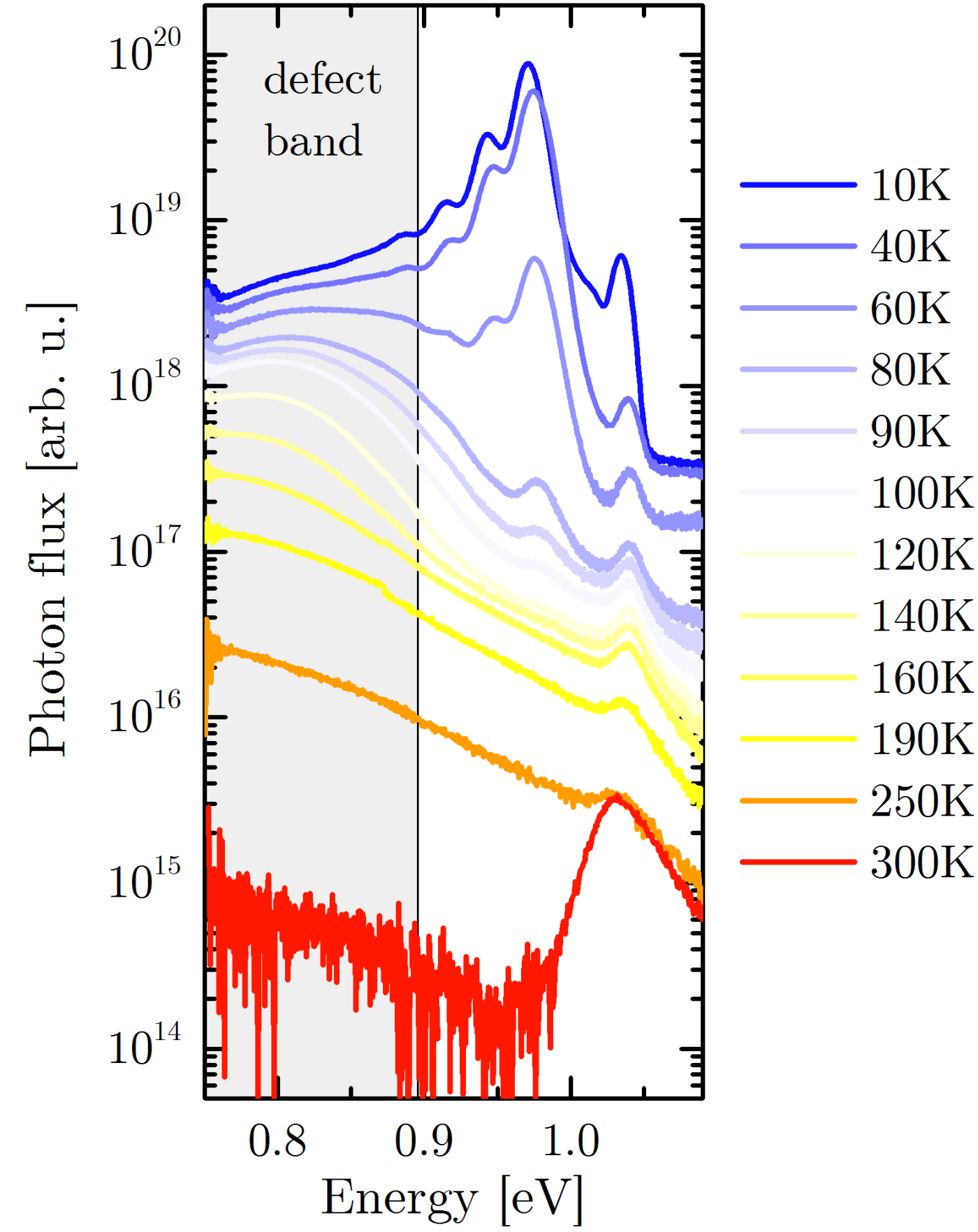
Shallow defects

- low temperature photoluminescence (10K)



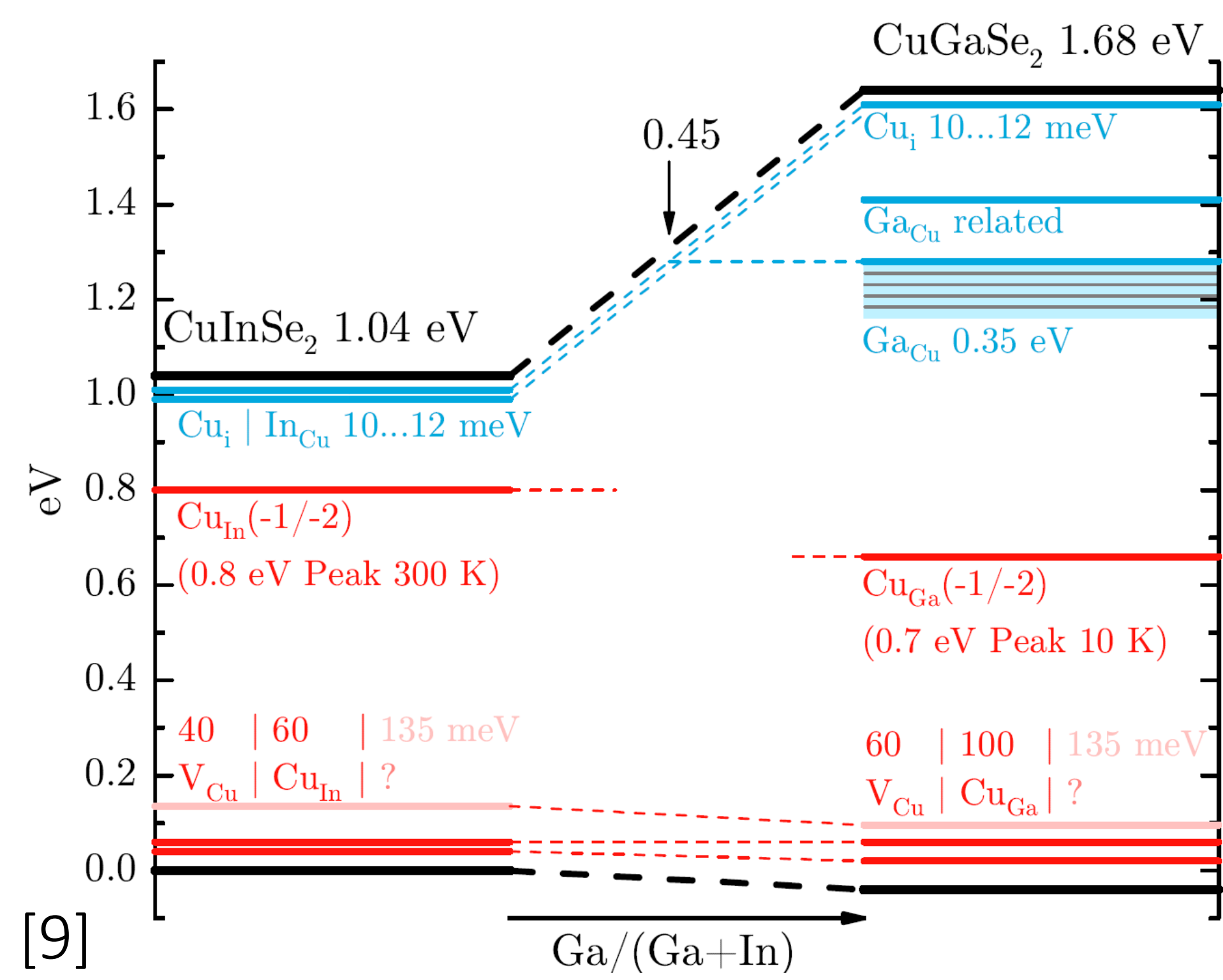
- D1**: shallow donors 8-14 meV (CISe/CGSe)
- A1**: stoichiometric low-Cu (40/60 meV)
- A2**: stoichiometric high-Cu (60/100 meV)
- A3**: CuInSe₂ with high selenium (135 meV)
CuGaSe₂ close to Cu/Ga = 1 (135 meV)

Deep 0.8 eV defect



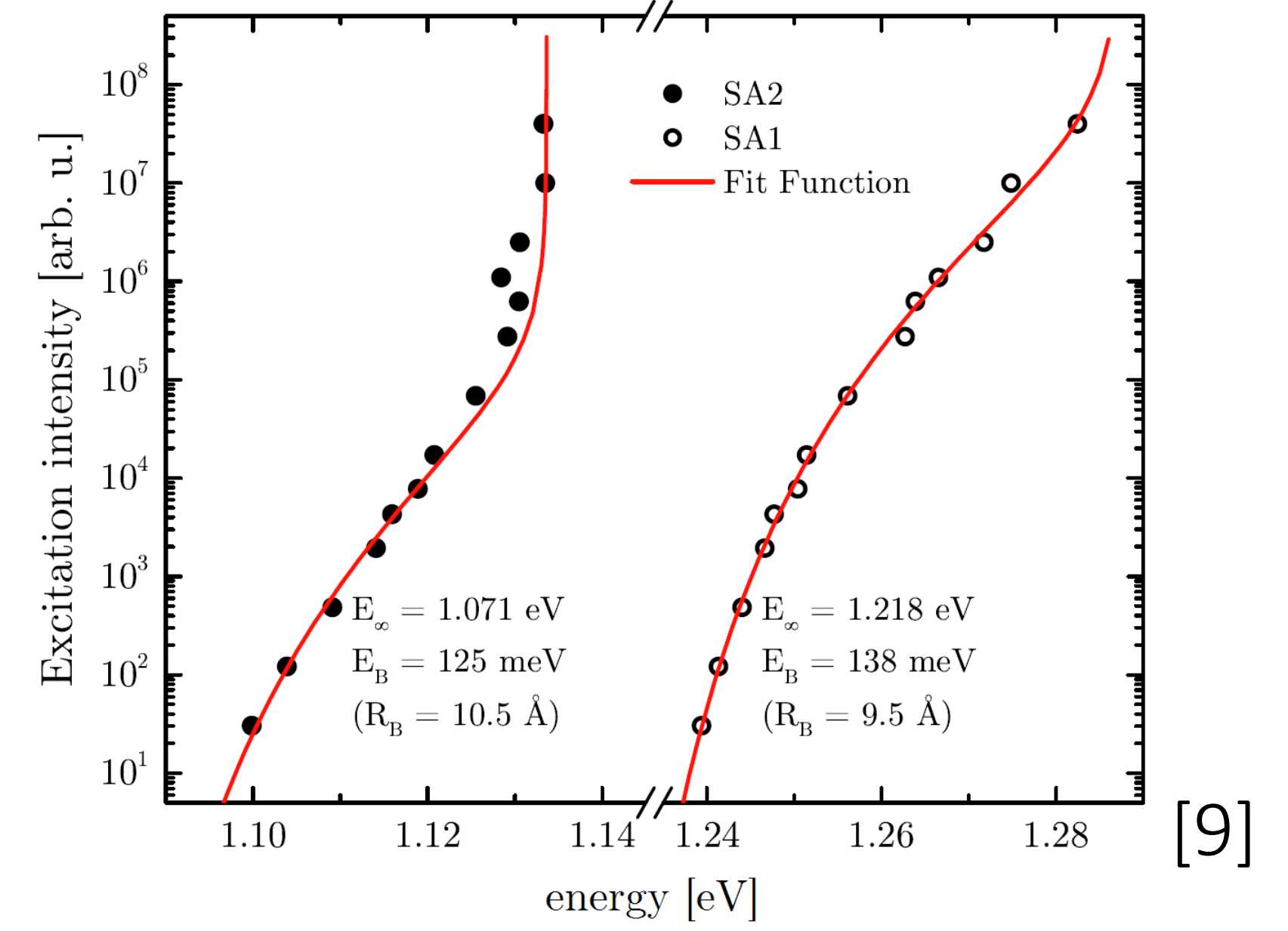
- 0.8 eV above valence band for varying GGI
- Broad density of states (ca. 0.1 eV)
- Always observed in Cu-rich compositions

Defect model in Cu(In,Ga)Se₂

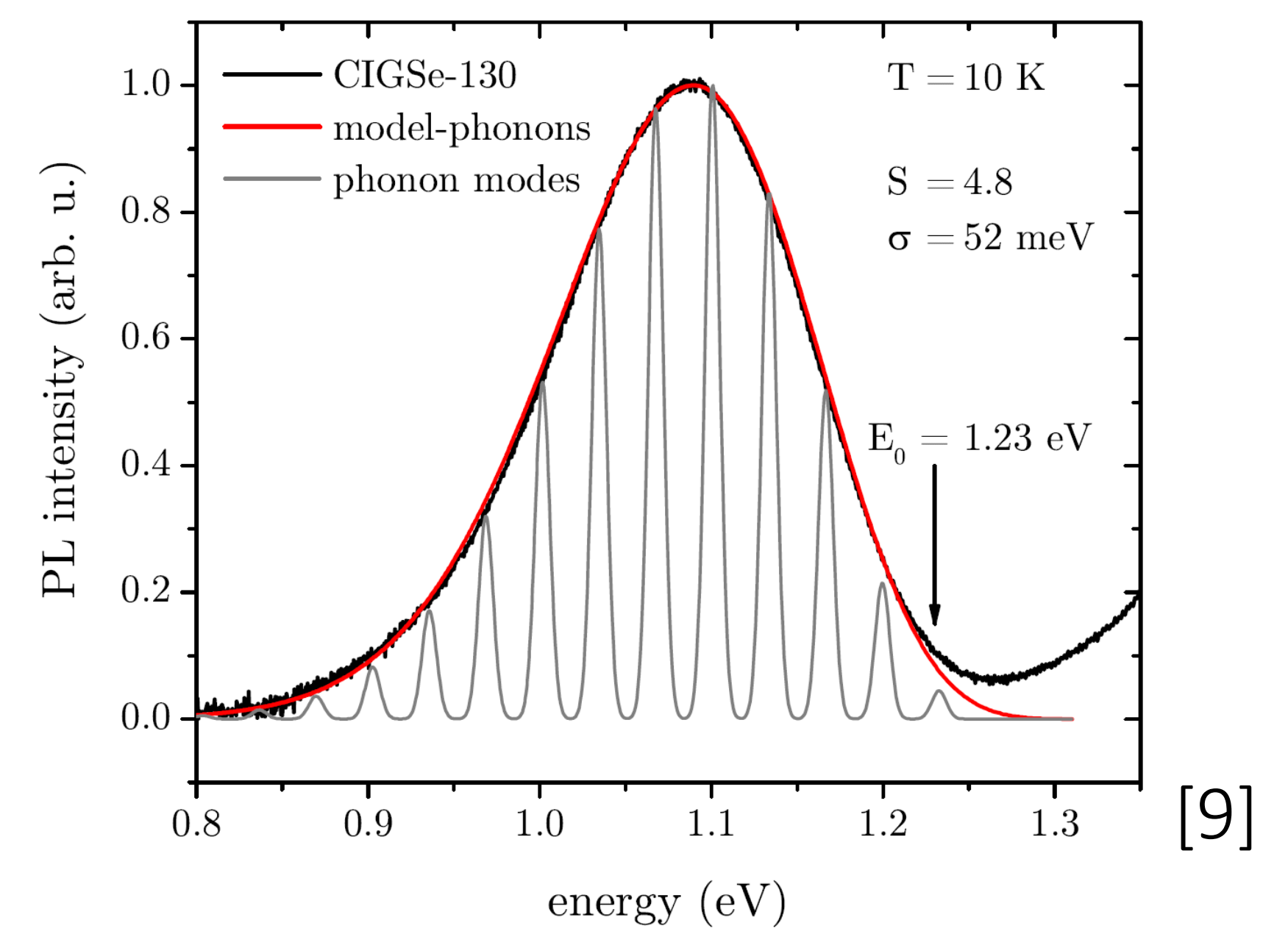


Deep 1.3 eV defect

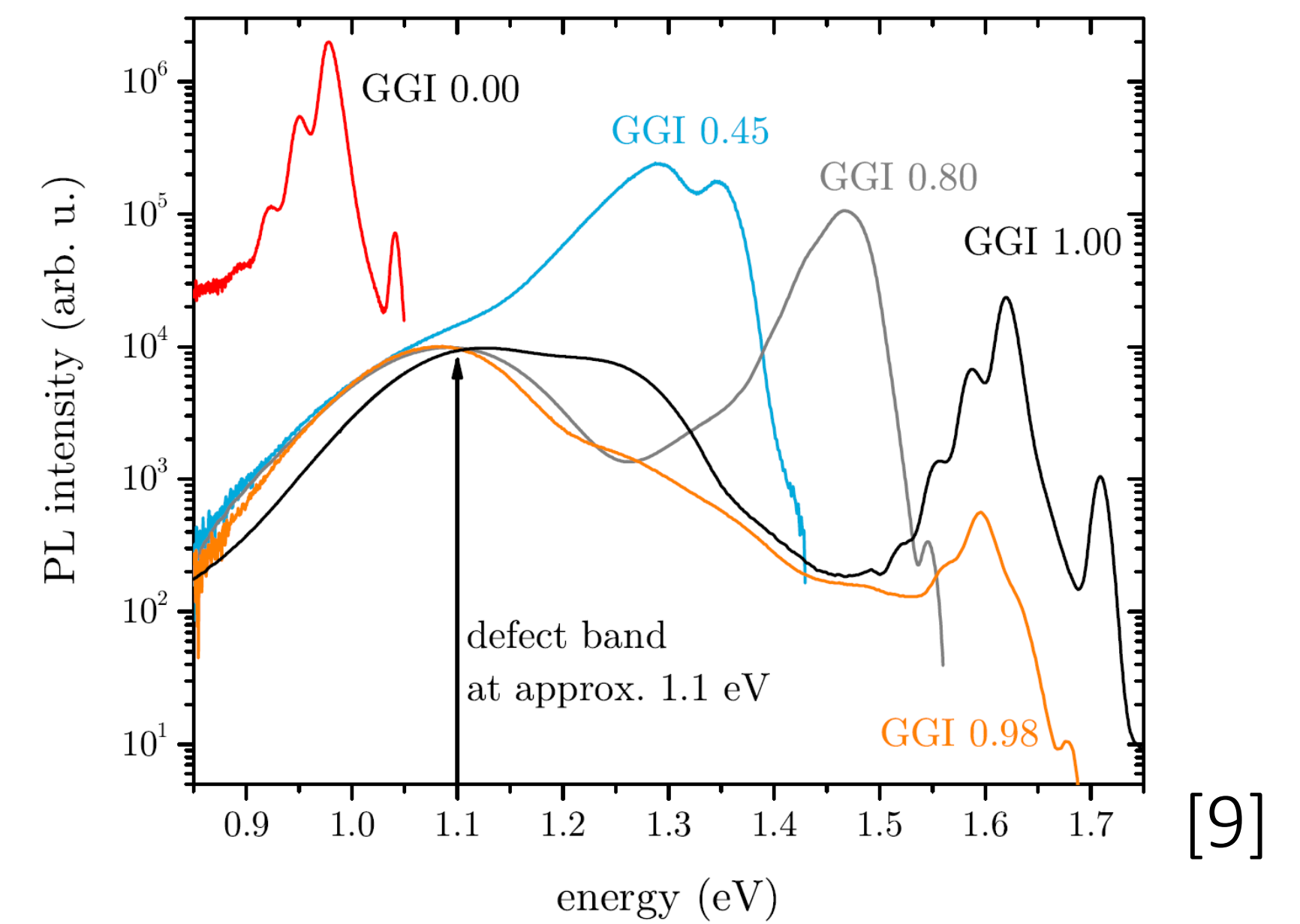
- Large blueshift of 2 deep bands in CuGaSe₂
→ Donor-acceptor pairs with shallow accept.



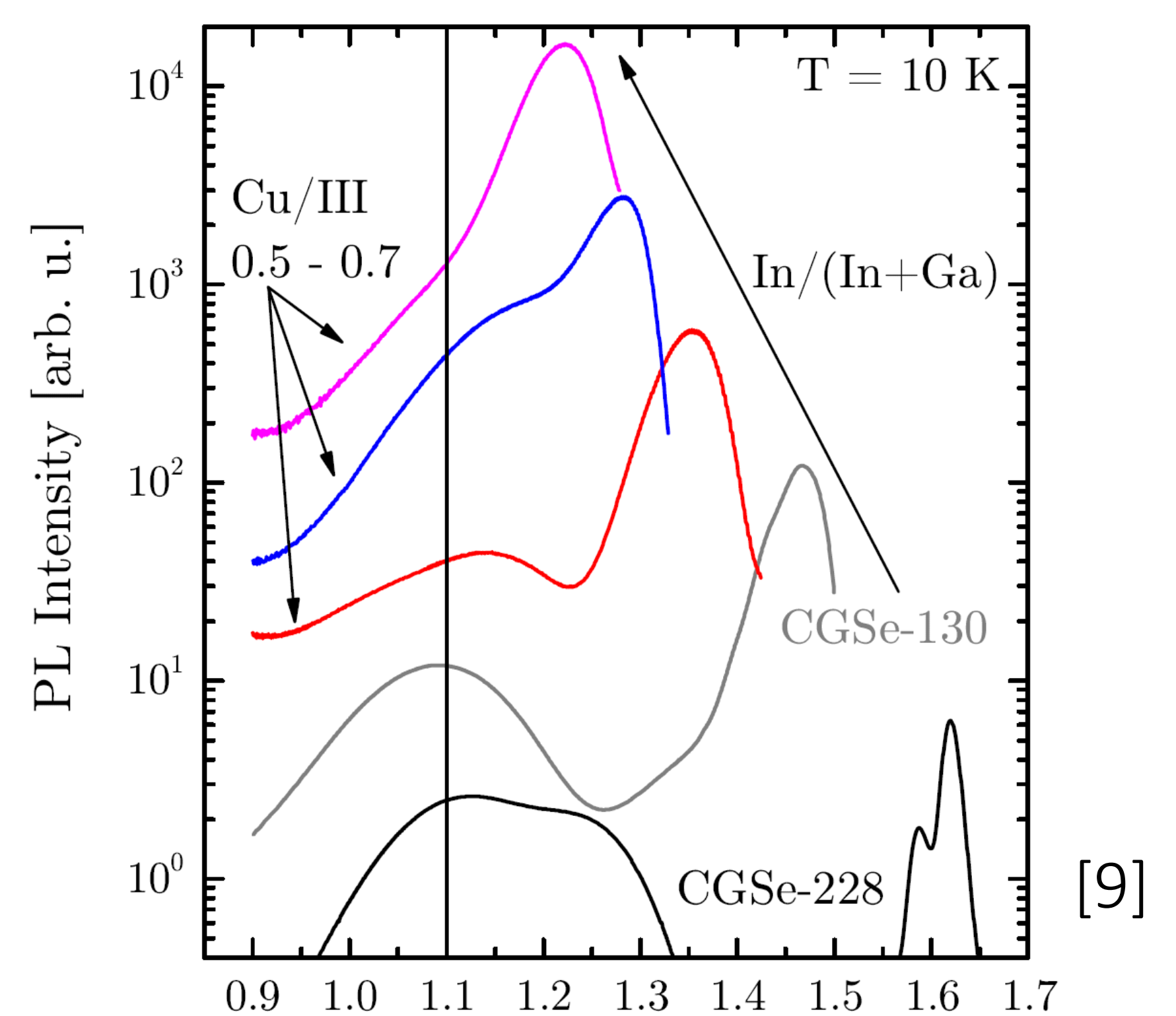
- With 20% of indium: single deep band
→ Determination zero-phonon line 1.23 eV
→ Deep donor-like defect around 1.3 eV



- 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



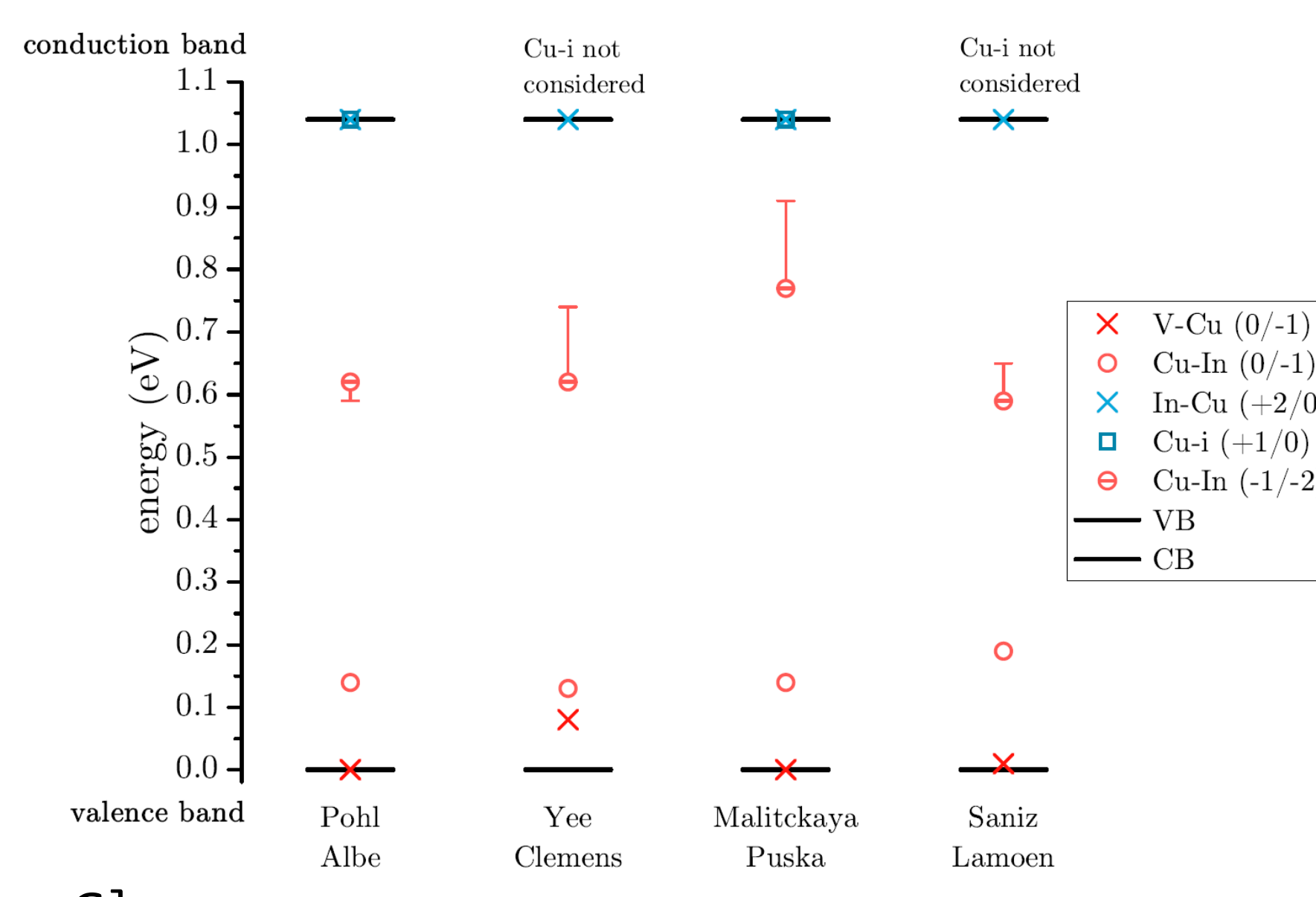
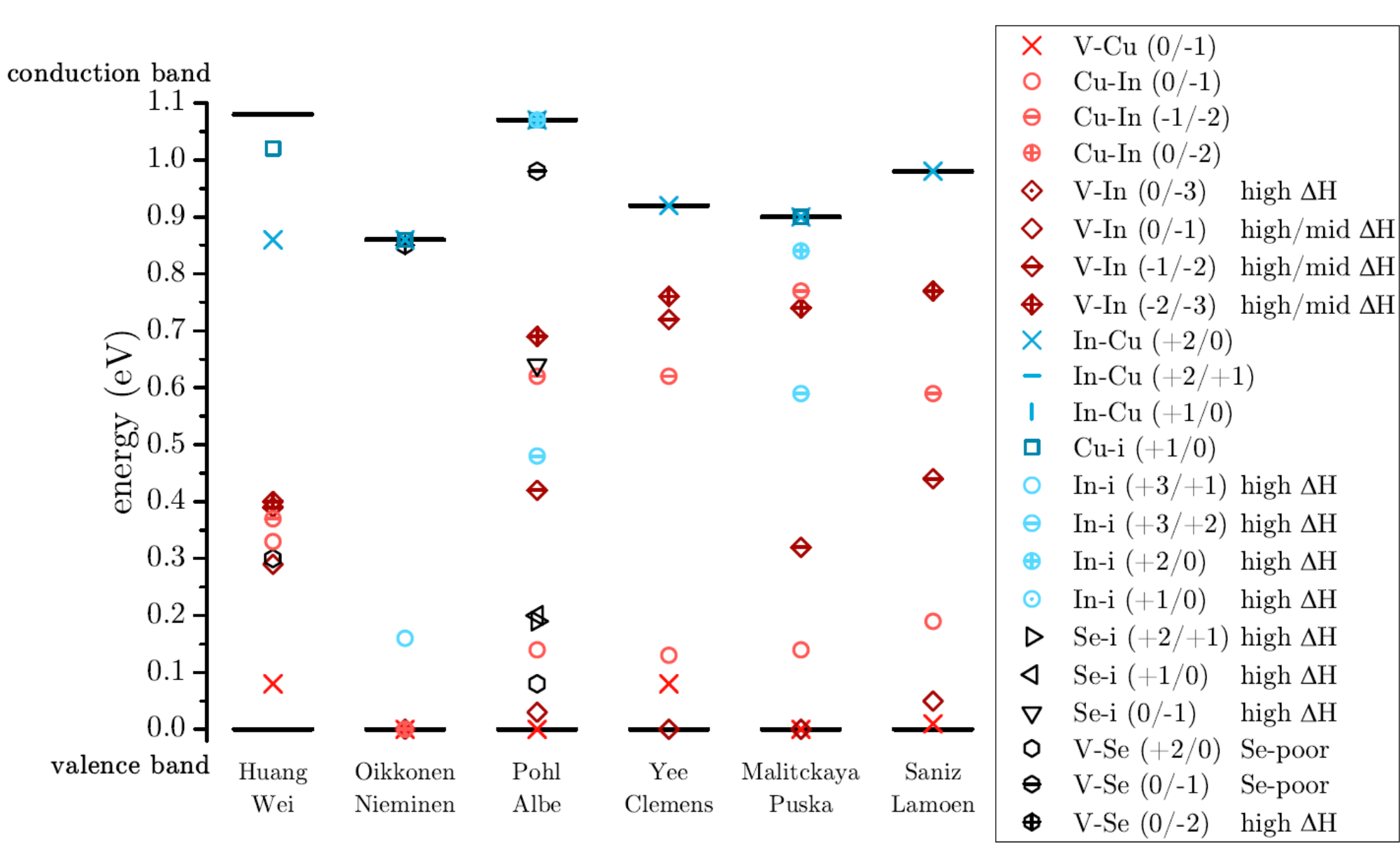
Defects from Theory

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



[1 – 6]

Literature

- [1] Huang/Wei, JPV 4, 2014
[2] Oikkonen/Nieminen, JPH 26, 2014
[3] Pohl/Albe, PRB 87, 2013
[4] Yee/Clemens, PRB 92, 2015
[5] Malitckaya/Puska, AEM, 2017
[6] Saniz/Lamoen, PCCP 22, 2017
[7] Siebentritt et. al., SEMSS 119, 2013
[8] Babbe/Siebentritt, under review
[9] Spindler, PhD Thesis, 2018

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