First-principles study of intrinsic point defects and hydrogen impurities in the earth-abundant solar absorber Zn_3P_2

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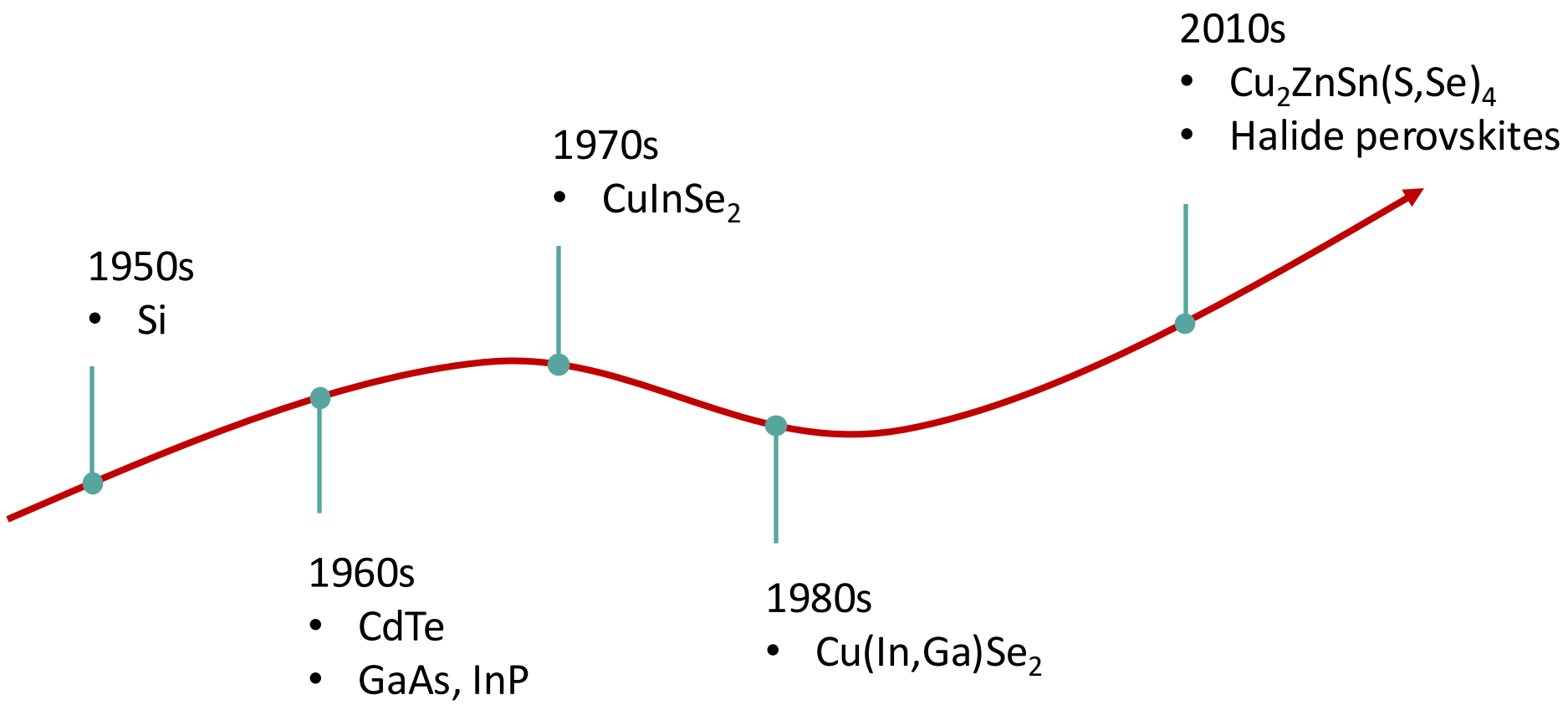
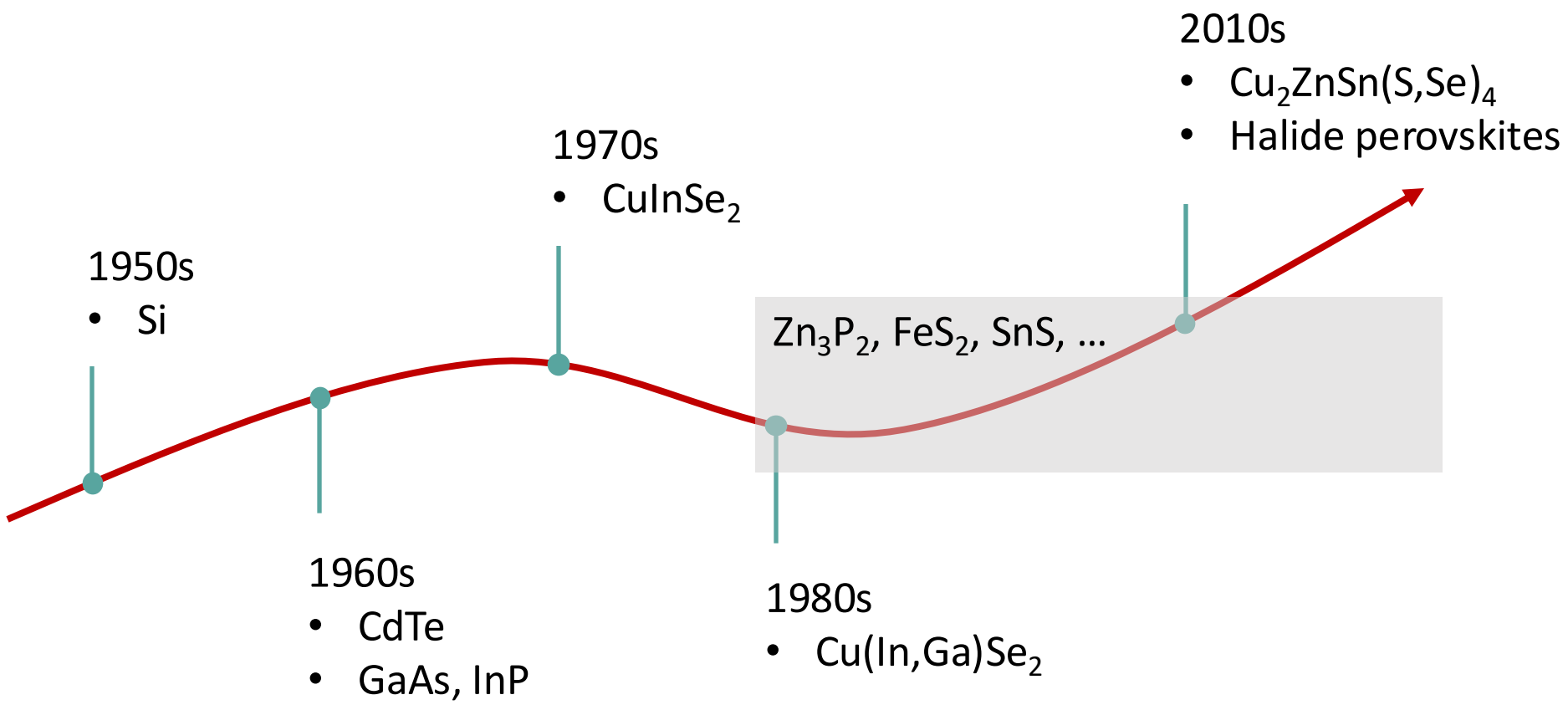
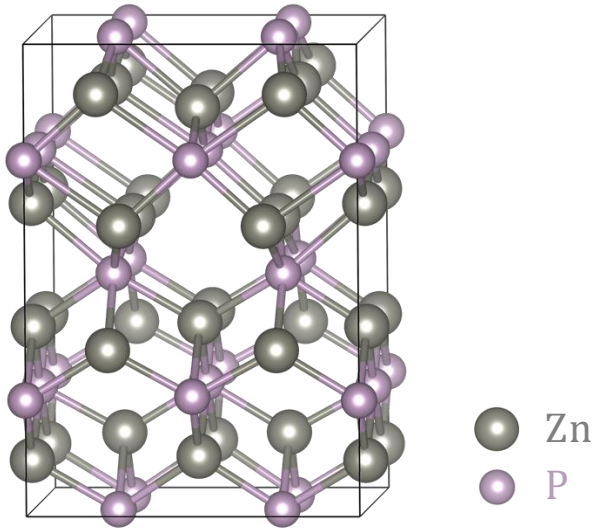
Solar cell absorbers

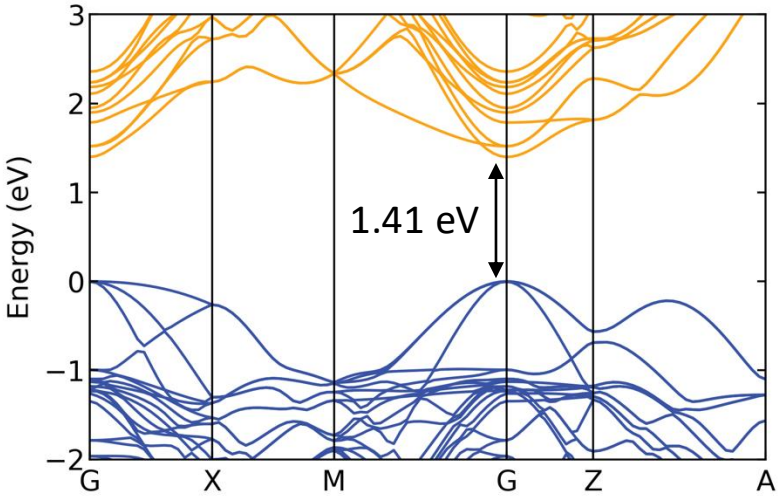


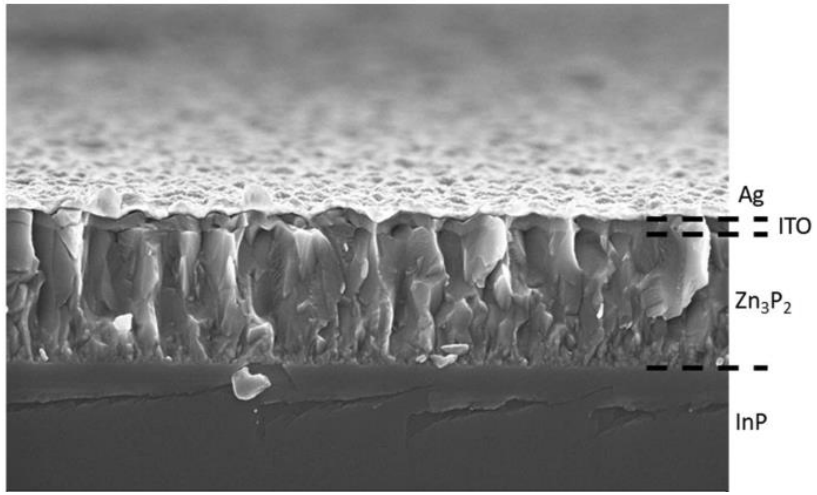
Solar cell absorbers



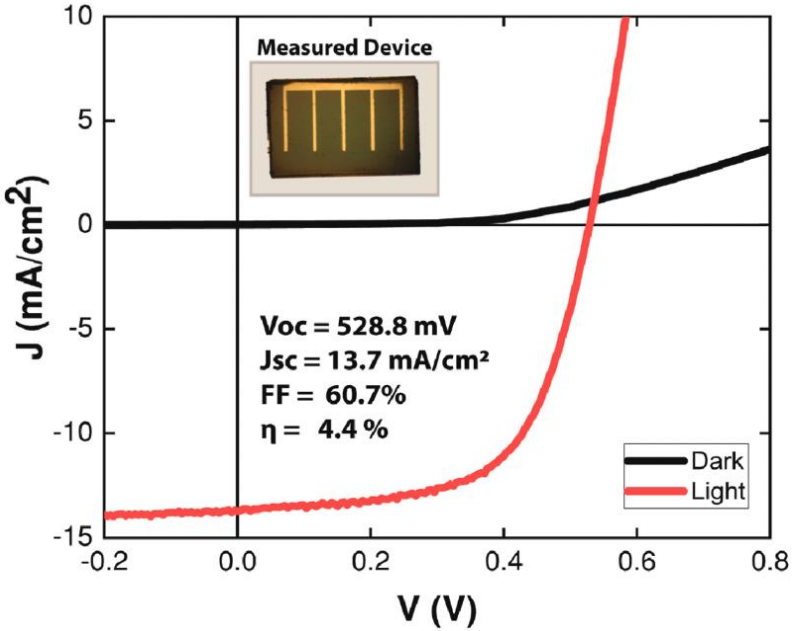
Zn_3P_2 solar cells







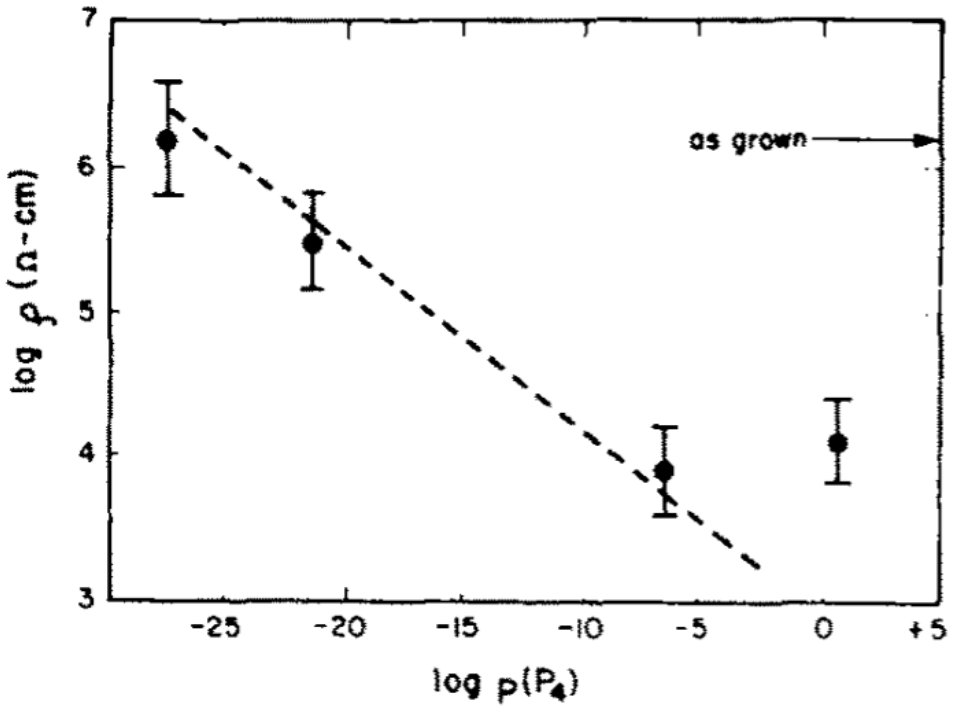
p-Zn_3P_2/n-InP junction

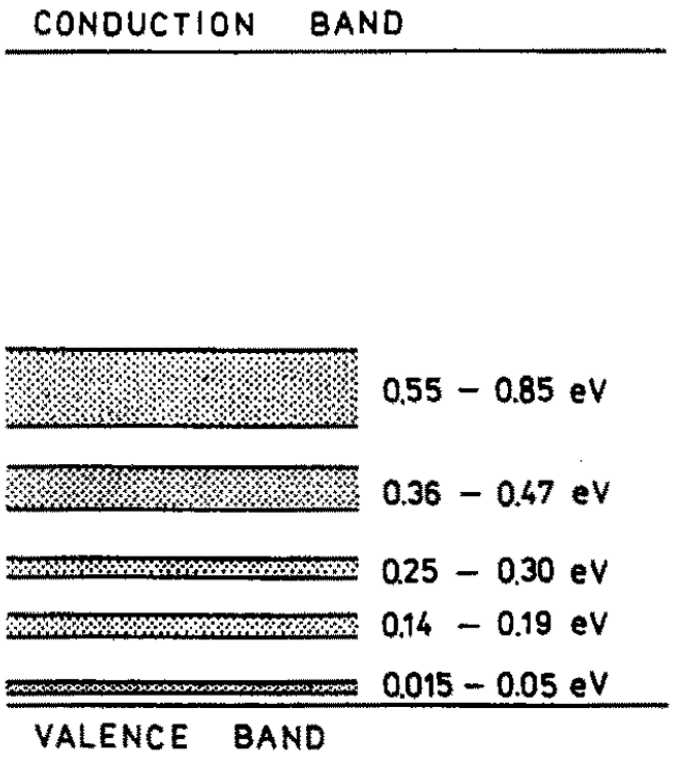


Paul *et al.*, *Sol. Energy Mater. Sol. Cells*, **256**, 112349 (2023)

Zn_3P_2 solar cells — Future optimizations

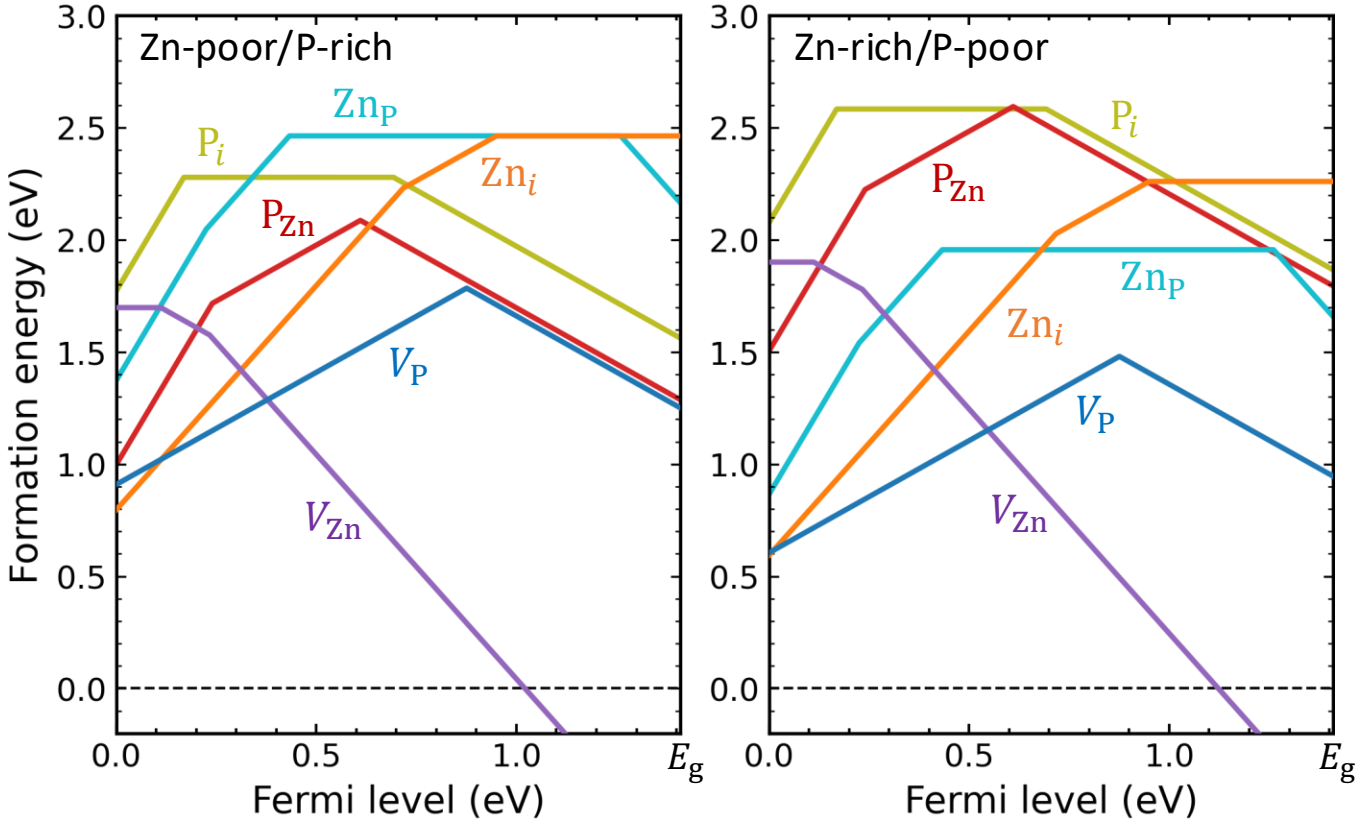
- Suitable n-type buffer to form pn junction with p-type Zn_3P_2
- Control of point defects and doping in the Zn_3P_2 absorber





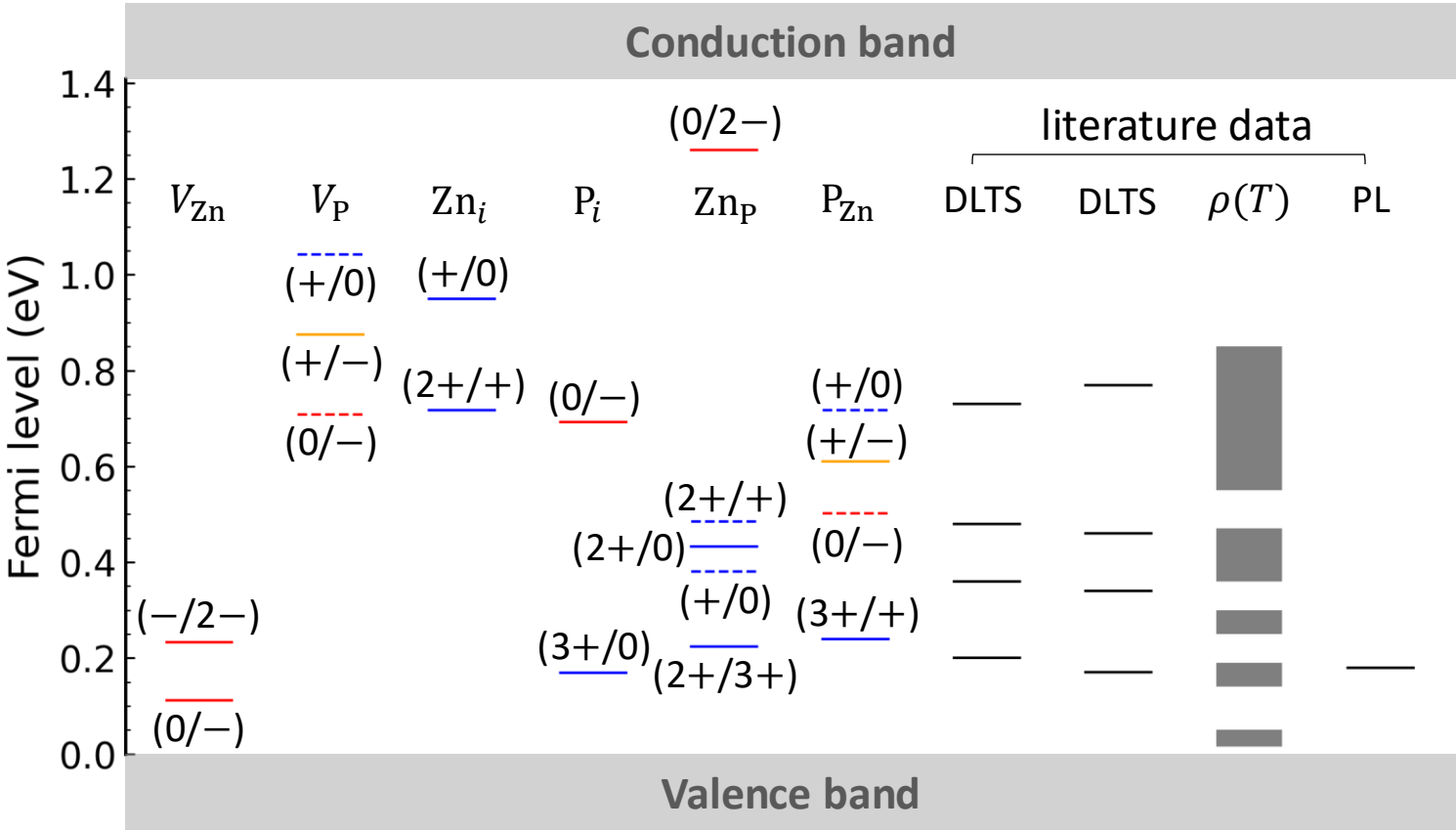
Catalano and Hall, *J. Phys. Chem. Solids*, **41**, 635 (1980)
Misiewicz, *J. Phys. Chem. Solids*, **41**, 635 (1980)

Intrinsic point defects in Zn_3P_2



- Most defects act as compensating centers in *p*-type Zn_3P_2
- P_i has a very deep acceptor behavior $\Longrightarrow$ unlikely contribute to *p*-type doping
- V_{Zn} is likely to be the source of *p*-type conductivity in as-grown Zn_3P_2
- Zn-poor/P-rich conditions $\Longrightarrow$ more V_{Zn} & less compensation

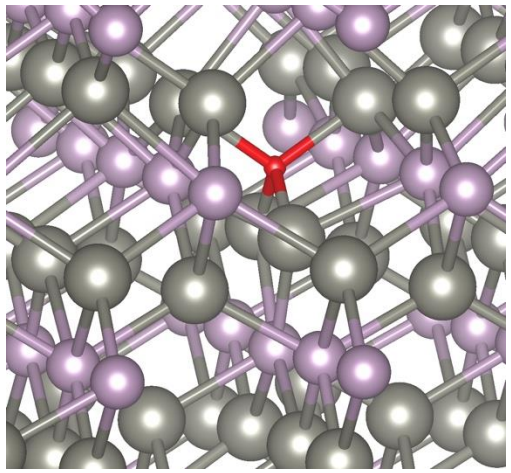
Defect levels



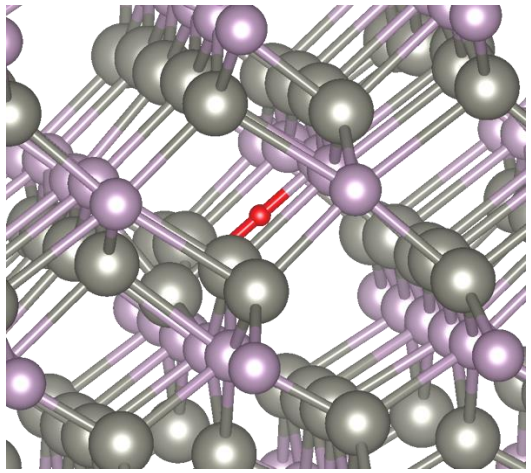
- Most defect levels are deep, especially those of V_P, Zn_i, P_i, and P_{Zn}
- Nonstoichiometric, P-rich Zn_3P_2 samples $\Longrightarrow$ more deep levels from P_{Zn} and P_i

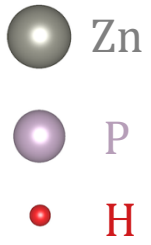
Hydrogen impurities in Zn_3P_2

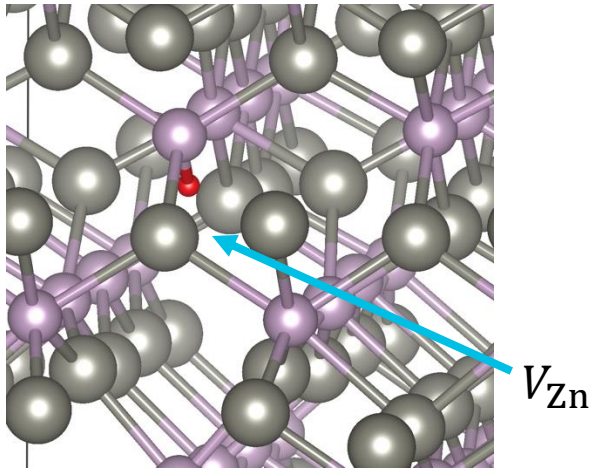
H_i^0 & H_i^-



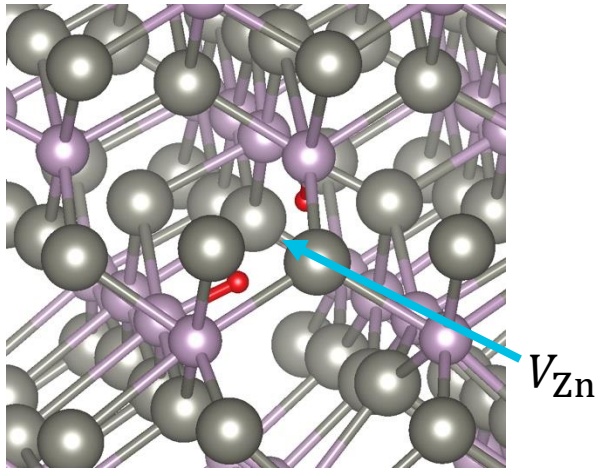
H_i^+



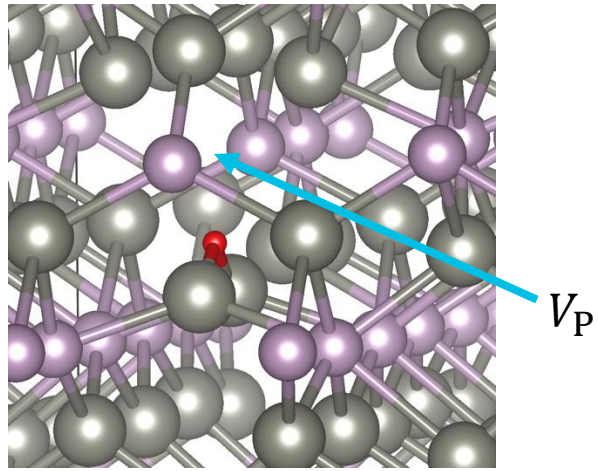




$H + V_{Zn}$

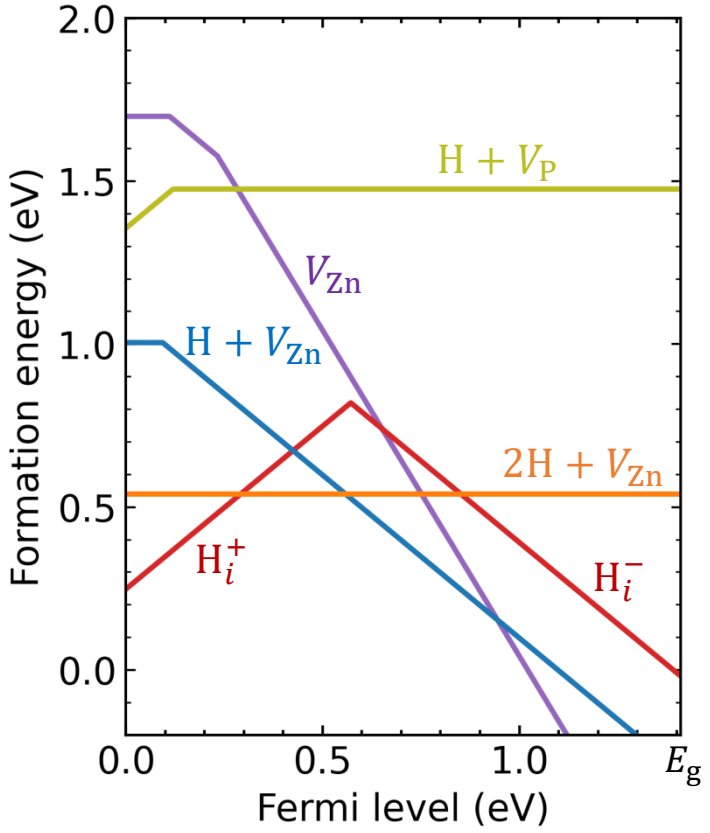


$2H + V_{Zn}$



$H + V_P$

Hydrogen impurities in Zn_3P_2



- Hydrogen is likely to form H_i^+ and complexes with V_{Zn} in *p*-type Zn_3P_2
  - H_i contributes to compensation
  - $H + V_{Zn}$ shallow acceptor
  - $H + 2V_{Zn}$ electrically inactive

Conclusions

- Most intrinsic defects are compensating centers in *p*-type Zn_3P_2 and have deep levels in the band gap
- V_{Zn} rather than P_i is likely the source of *p*-type conductivity in as-grown Zn_3P_2
- While Zn-poor/P-rich growth conditions are needed to enhance *p*-type conductivity, such conditions will facilitate the formation of P_{Zn} and P_i
  - good PV performance not guaranteed for nonstoichiometric, P-rich Zn_3P_2 films
- Hydrogen in Zn_3P_2 is likely to form H_i^+ and complexes with the V_{Zn} acceptors

Yuan, Xiong, and Hautier, *J. Mater. Chem. A*, 2023
(in press)

Acknowledgements

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Thank you for your attention!