Localized states due to oxygen in II-VI semiconductors

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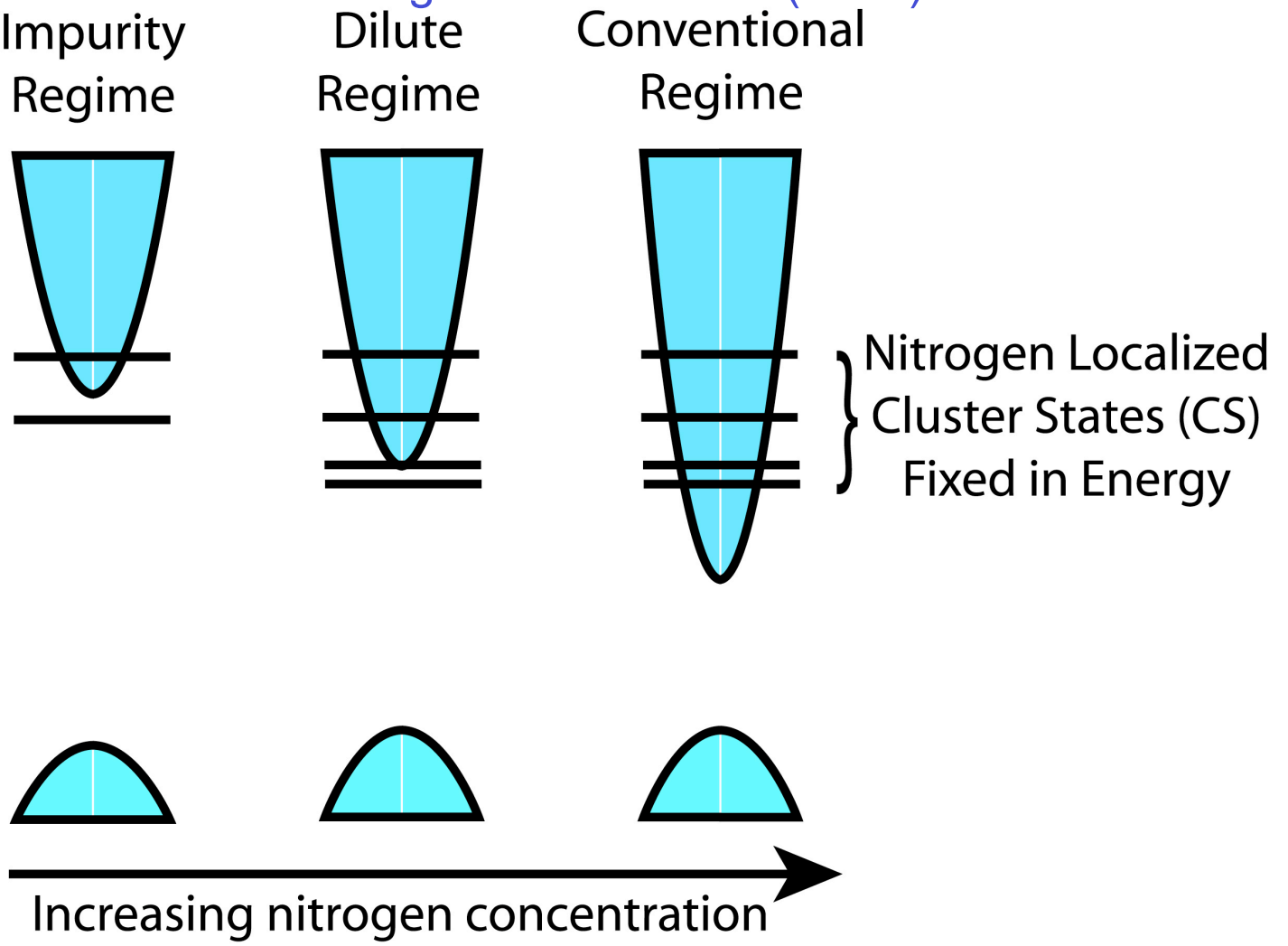
Localized-Delocalized Transition in GaAsN

Kent and Zunger PRL **86** 2613 (2001)



Localized states result in large bowing, anomalous pressure coefficients, effective mass....

The questions I will address

Do oxygen cluster states occur in II-VI materials?

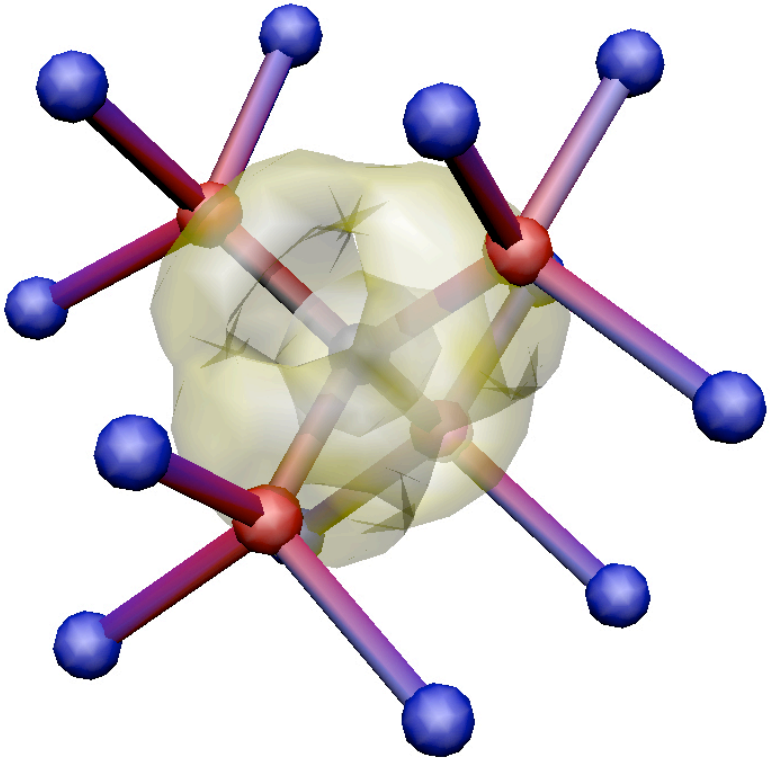
What are their properties?

Computational methodology

1. Isolated impurity calculations
   - ZnTe:O, ZnSe:O,ZnS:O
   - CdTe:O, CdSe:O,CdS:O
2. Fully relaxed self-consistent density functional calculations
   - PAW and norm-conserving pseudopotential
   - Up to 216 atom supercells (~18x18x18A)
   - Local density approximation
3. Electronic states characterised using:
   - Calculated localisation (charge within sphere) $Q = \int_0^R |\Psi|^2 dr$
   - Density of states under hydrostatic pressure
   - "Majority representation" G/L/X

     Wang *et al.* PRL **80** 4725 (1998)

Localization in GaP:N



Nitrogen localized a_1(N)

4096 atom EPM calculation

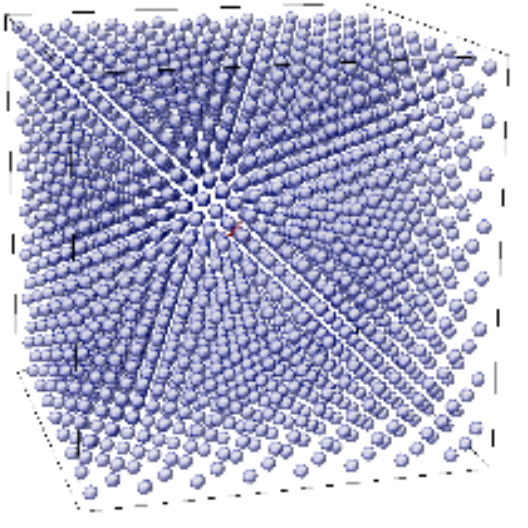
50% of charge with ~5A

In GaP:N (0.01%):

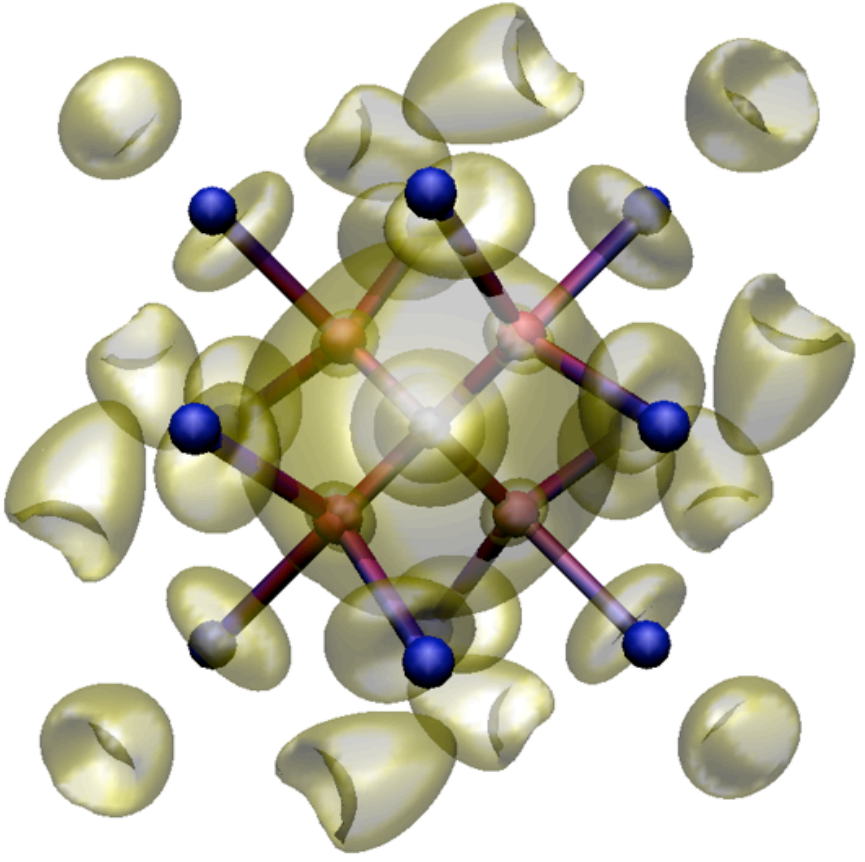
Level ~30 meV below CBM

Introduces Γ character - "direct gap"

Delocalized wavefunction



Localized states in ZnTe:O



Oxygen localized a1(O)

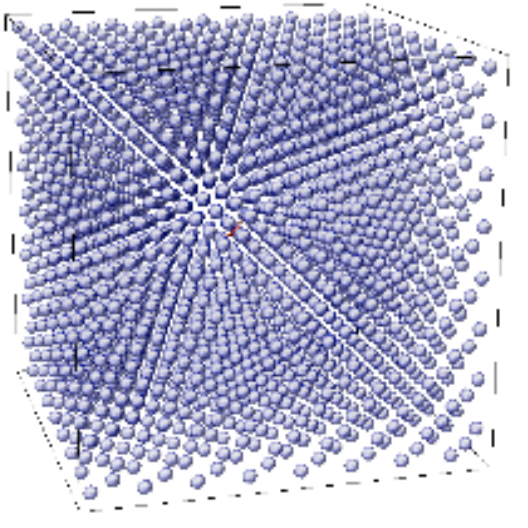
216 atom LDA-DFT
50% of charge within ~6A

In ZnTe:O:

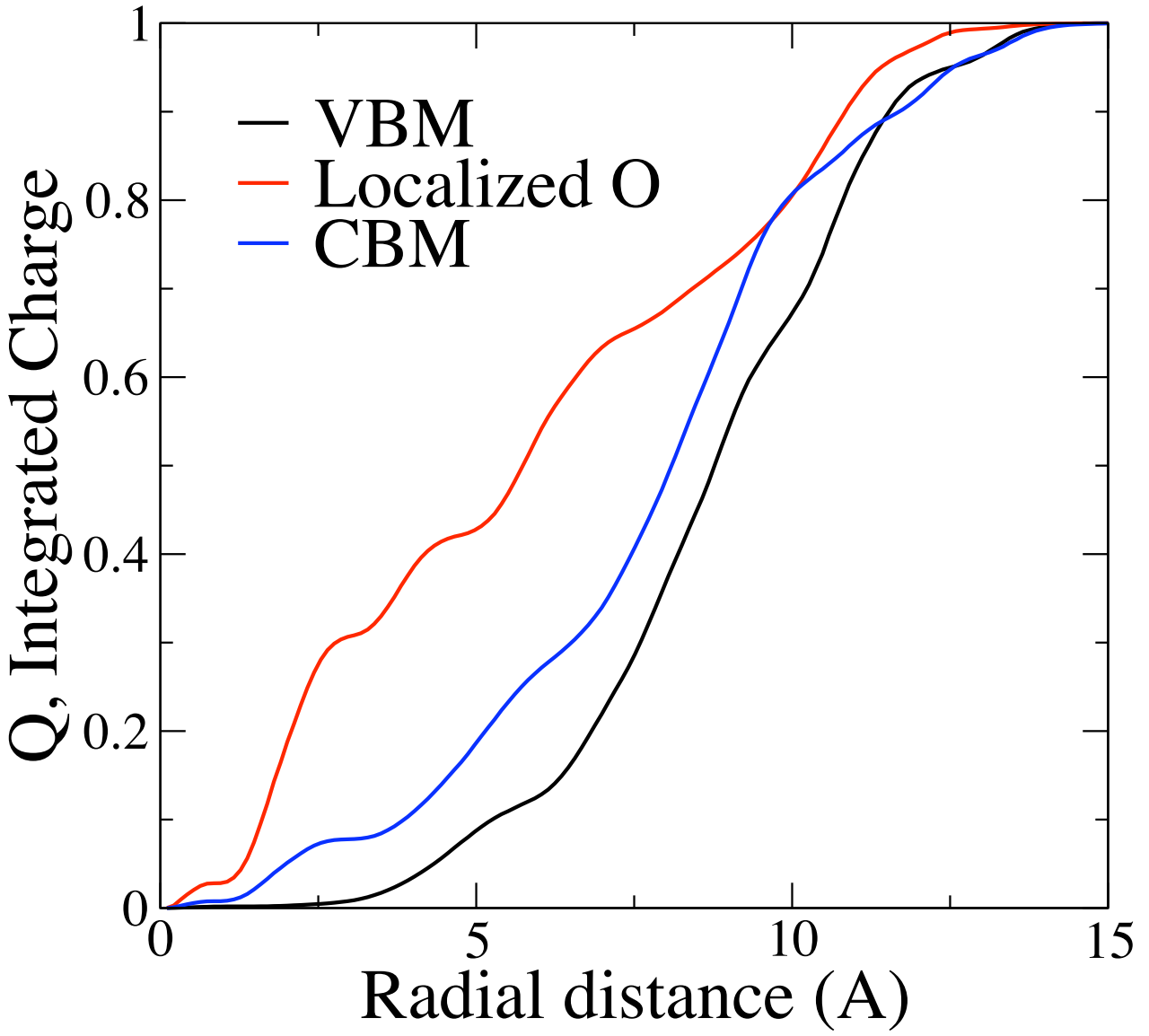
Level ~0.6 eV below conduction band edge.

"Deeper" version of GaX:N

Delocalized wavefunction

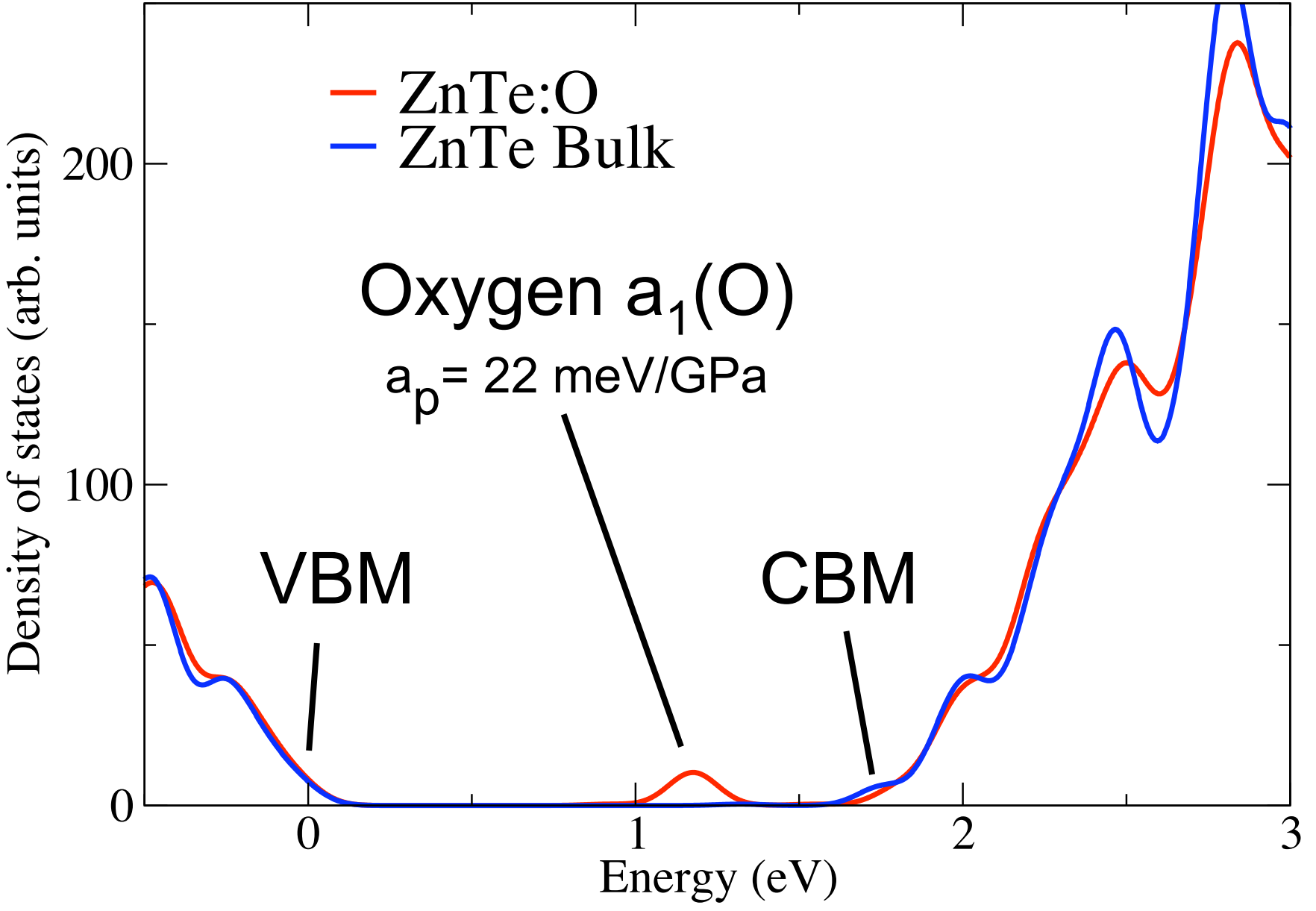


Localization in ZnTe:O



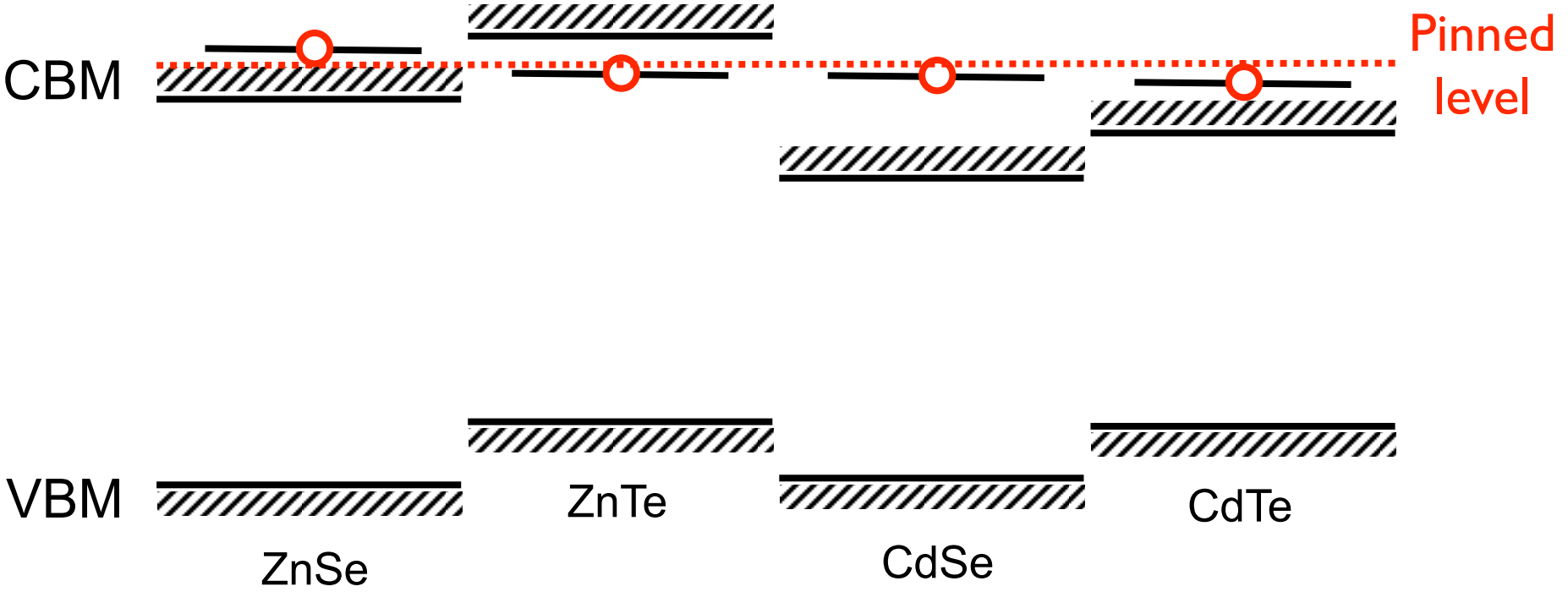
More localised than for GaAs:N due to larger energetic separation between states. Kent and Zunger PRB **64** 115208 (2001)

DOS and Pressure effects in ZnTe:O



Summary of II-VI:O results

(Not to scale)

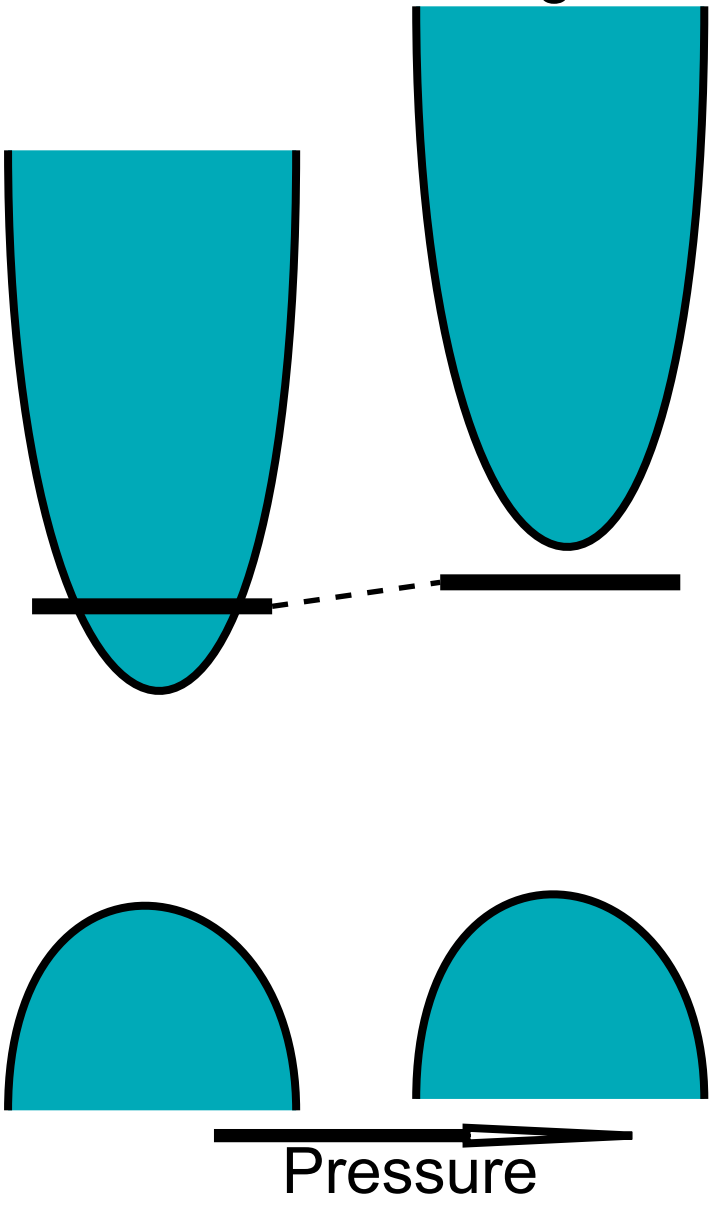


Wei APL **72** 2011 (1998) + Llandolt Bornstein

1. Localization always found:
   gap state only for ZnTe, resonant states in other cases.
2. O level *approximately* pinned in energy across material

Pressure effects

Resonant states emerge into the gap with hydrostatic pressure



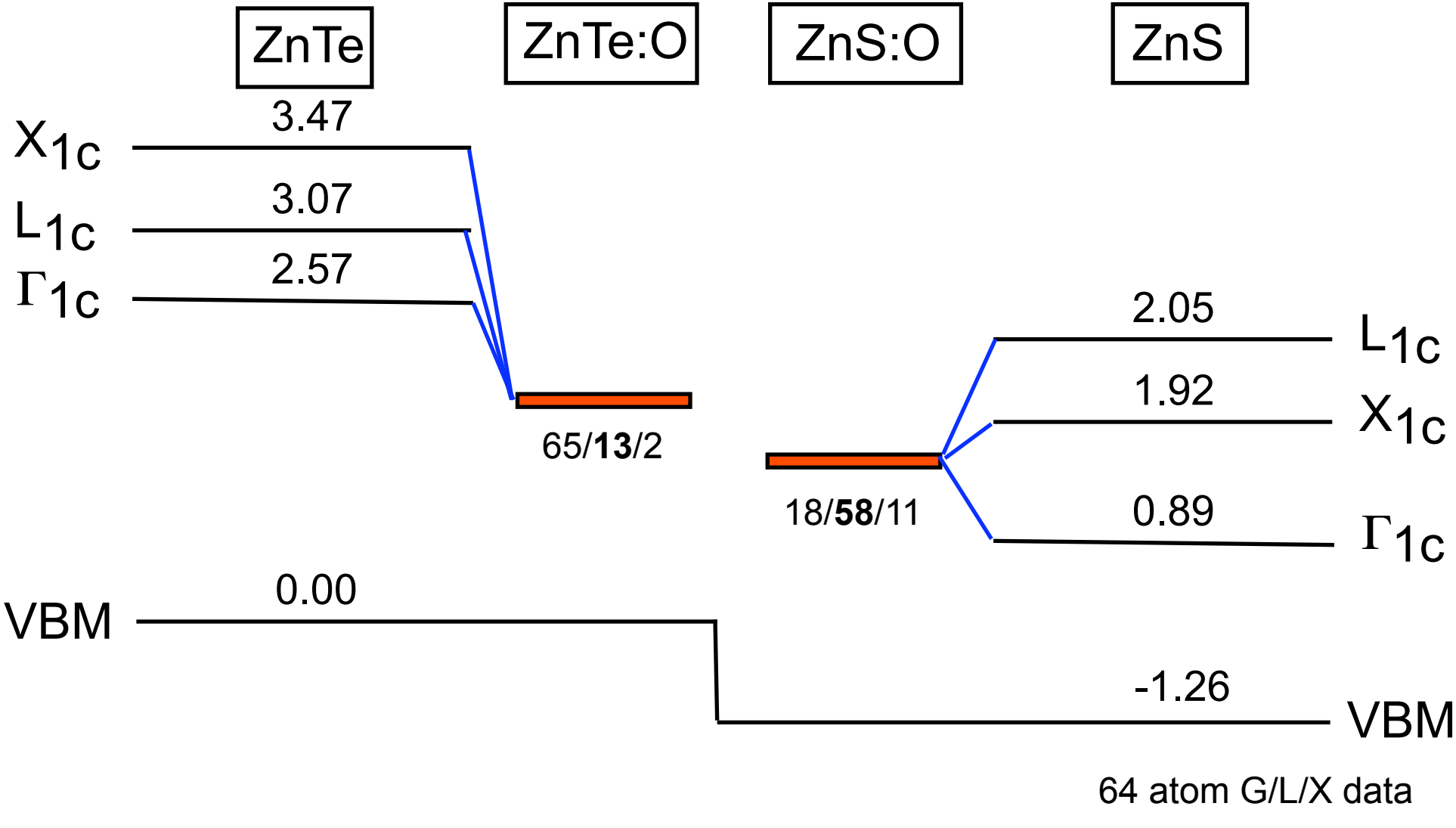
"Few GPa emergence"

Band edge: Large pressure coefficient
O level: Small pressure coefficient

All O levels can be observed under sufficient pressure

Character of localized states

Gamma and L-point states strongly coupled



64 atom G/L/X data

Summary

- O causes localized states in II-VI
  - ZnTe:O level in gap
  - Other materials: resonant level
- Similar to N levels in III-Vs
  - Small pressure coefficient
  - O pairs, clusters (deeper)
  - Large, composition dependent bowing
- Many band phenomenon:
  - G,L-states strongly coupled