Presentation on:
Band Anticrossing in highly mismatched III-V semiconductor alloys

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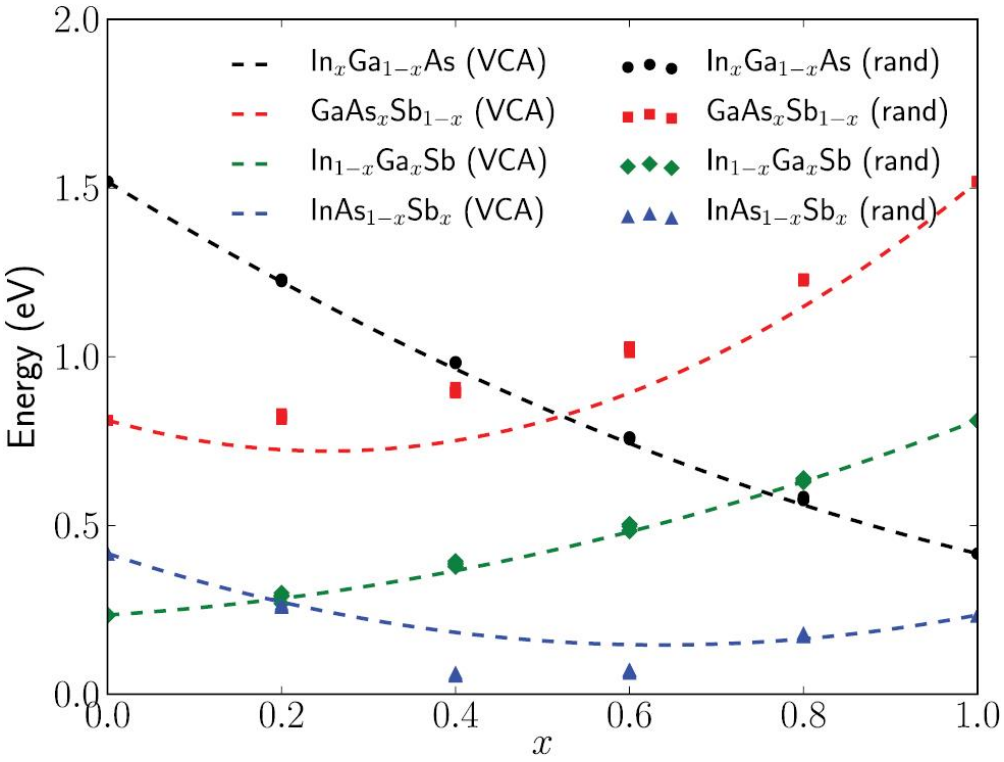
Condensed Matter Journal Club

April 24th, 2018

Virtual Crystal approximation (VCA)

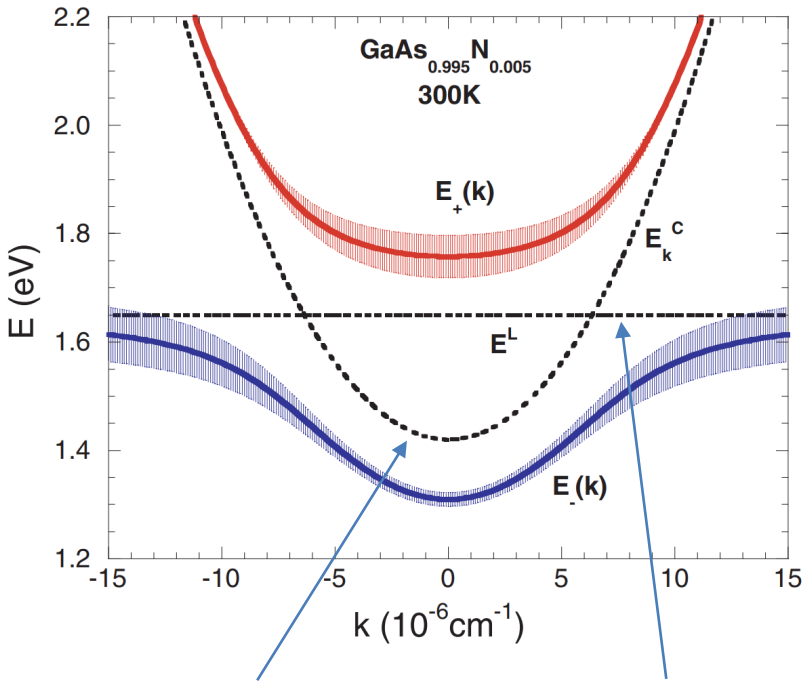
- Linear interpolation between properties of end point materials
  - Bowing parameter
- Highly mismatched alloys (HMA) – differ drastically from predictions of VCA
- III-V_{1-x}-N_x
  - highly electronegative nitrogen substitutes group V anion
  - N and As electronegativity (Δ = 0.86)



M. O. Nestoklon *et al.*, Journal of Physics: Condensed Matter **28** (30), 305801 (2016).

Band Anticrossing Model (BAC)

- W. Shan *et al.*, Physical Review Letters **82** (6), 1221 (1999). – for GaInNAs
- Restructuring of conduction band
  - Anticrossing interaction between highly localized A_1 states of the substitutional N and the extended states of the host material
  - $E^C(k)$ is energy dispersion of lowest conduction band of host
  - $E^L(k)$ is energy of localized states from substitutional N atoms
  - Coupling strength is given by V
  - E_+ and E_- are the new sub-bands



GaAs Conduction Band

Nitrogen A_1 level

$$E_{\pm}(k) = \frac{1}{2}\left\{[E^C(k) + E^L] \pm \sqrt{[E^C(k) - E^L]^2 + 4V^2 \cdot x}\right\}, \quad (1)$$

Band Anticrossing Model (BAC)

- Basic form – degenerate perturbation theory applied to a system of localized states and extended states

- Similar to s-d exchange interaction model – single site Anderson model – magnetic impurities in metallic hosts
  - Electron system in delocalized part of the metal described in terms of band theory
  - Localized level – provided by the d-shell electrons of the impurity

- Many-impurity Anderson model
  - Electronic properties of semiconductors with deep-level transition-metal impurities

Theory

- Described like the many-impurity Anderson model
- Here we consider an interaction between the localized states $|L\rangle$ and the extended states $|\boldsymbol{k}\rangle$

$$H = \sum_{\mathbf{k}} E_{\mathbf{k}}^{C} c_{\mathbf{k}}^{+} c_{\mathbf{k}} + \sum_{j} E_{\mathbf{j}}^{L} d_{\mathbf{j}}^{+} d_{\mathbf{j}}$$

$$+ \frac{1}{\sqrt{N}} \sum_{j,\mathbf{k}} (\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{j}} V_{\mathbf{kj}} c_{\mathbf{k}}^{+} d_{\mathbf{j}} + \mathrm{h.c.}),$$

- Anderson Model
  - Electrons with energy dispersion E_k^C
  - Electrons localized on impurity sites
  - Change in single electron energy due to dynamical mixing

- Hybridization strength - V_{kj}
- With only a single impurity, the model reduces to the original Anderson model

$$\langle \mathbf{k}|H_{\mathrm{HF}}|L\rangle = \frac{1}{\sqrt{N}} \sum_{l,j} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{l}} \int a^{*}(\mathbf{r}-\mathbf{l}) H_{\mathrm{HF}}(\mathbf{r}) \varphi_{L}(\mathbf{r}-\mathbf{j})\,\mathrm{d}\mathbf{r}$$

$$= \frac{1}{\sqrt{N}} \sum_{j} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{j}} \cdot \sum_{l} \mathrm{e}^{\mathrm{i}\mathbf{k}(\mathbf{l}-\mathbf{j})}$$

$$\times \int a^{*}(\mathbf{r}-\mathbf{l}) H_{\mathrm{HF}}(\mathbf{r}) \varphi_{L}(\mathbf{r}-\mathbf{j})\,\mathrm{d}\mathbf{r}$$

$$\equiv \frac{1}{\sqrt{N}} \sum_{j=\mathrm{l}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{j}} V_{\mathbf{kj}},$$

Theory

$$G_{\mathbf{kk}}(E) = \left[E - E^C_{\mathbf{k}} - \frac{V^2 x}{E - E^L - \mathrm{i}\pi\beta V^2 \rho_0(E^L)} \right]^{-1}$$

- Coherent potential approximation (CPA)
  - Used to find average coupling strength term V

- Solutions - 2 level eigenvalue-like problem
- Γ_L is the broadening of E^L in the single-impurity Anderson model

$$\begin{vmatrix} E^C_{\mathbf{k}} - E(\mathbf{k}) & V\sqrt{x} \\ V\sqrt{x} & E^L + \mathrm{i}\Gamma_L - E(\mathbf{k}) \end{vmatrix} = 0,$$

If Γ_L (broadening term) is 0, our solution reduces to the basic two level model

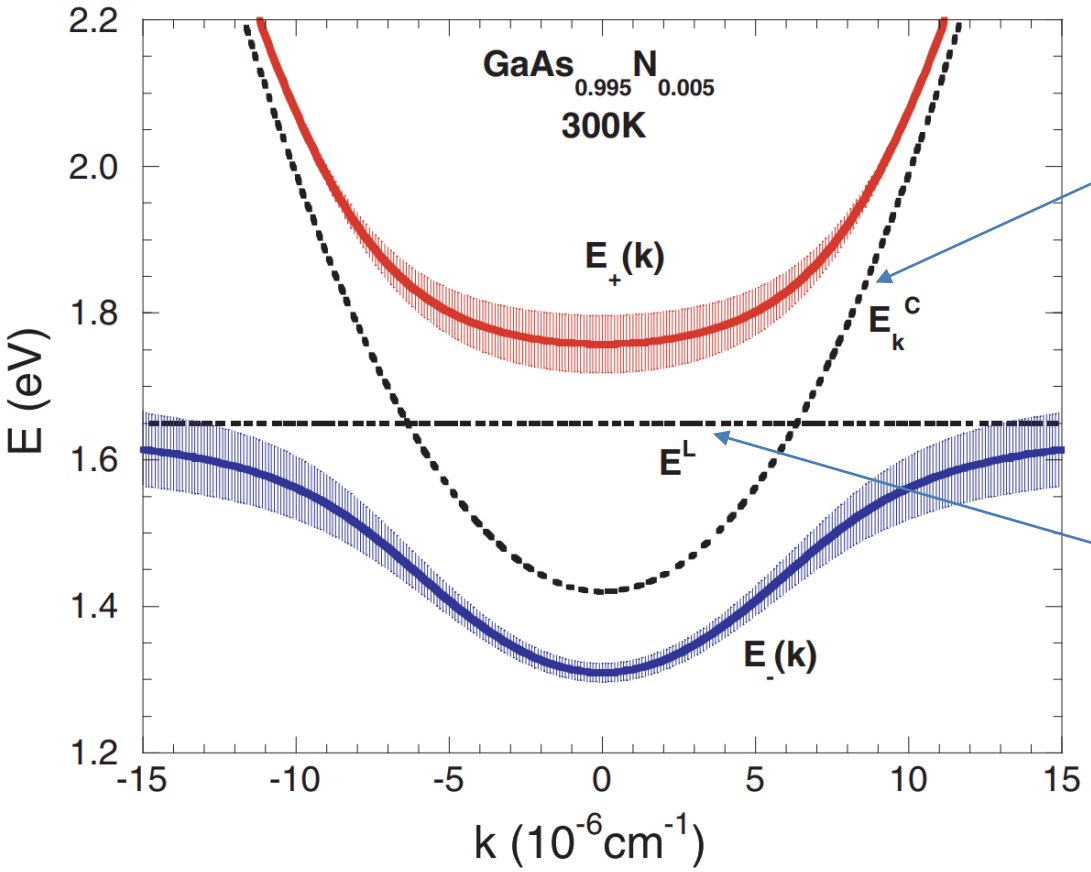
$$E_{\pm}(k) = \tfrac{1}{2}\left\{ [E^C(k) + E^L] \pm \sqrt{[E^C(k) - E^L]^2 + 4V^2 \cdot x} \right\},$$

If $\Gamma_L \neq 0$, but small

$$\tilde{E}_{\pm}(\mathbf{k}) \approx E_{\pm}(\mathbf{k}) + \mathrm{i}\Gamma_L \frac{\left[E_{\pm}(\mathbf{k}) - E^C_{\mathbf{k}}\right]}{\left[E_{\pm}(\mathbf{k}) - E^C_{\mathbf{k}}\right] + \left[E_{\pm}(\mathbf{k}) - E^L\right]}$$
$$\equiv E_{\pm}(\mathbf{k}) + \mathrm{i}\Gamma_{\pm}(\mathbf{k}),$$

$$\Gamma_{\pm}(\mathbf{k}) = |\langle L | E_{\pm}(\mathbf{k}) \rangle|^2 \cdot \Gamma_L.$$

Theory



GaAs Conduction Band

Nitrogen A_1 level

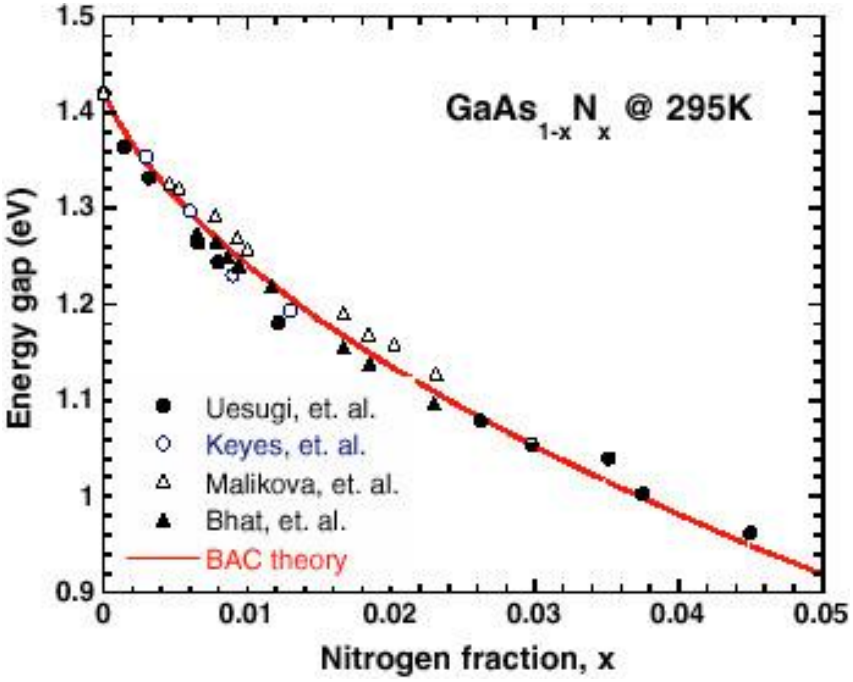
Dispersion given by

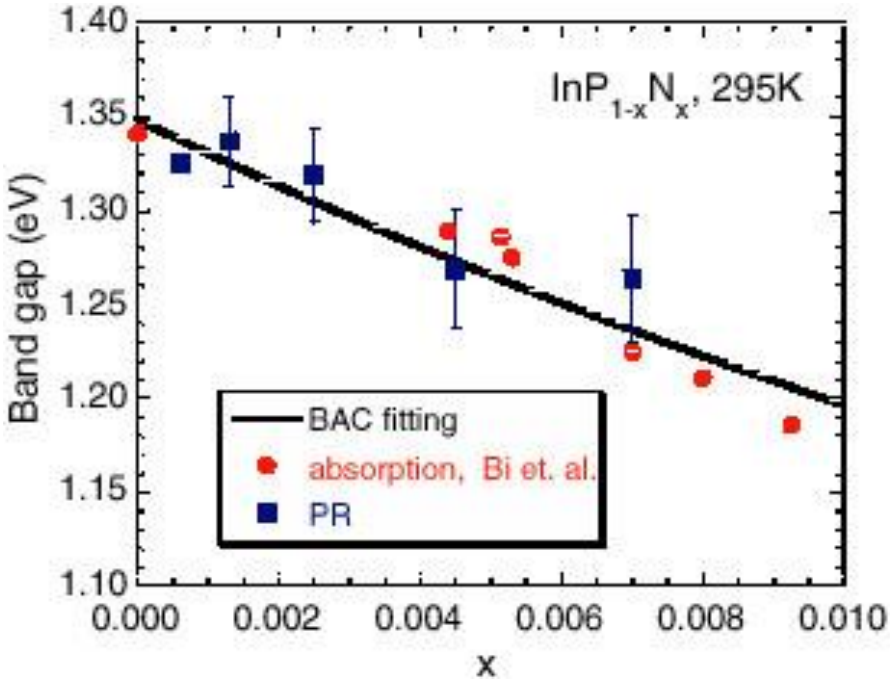
$$E_{\pm}(k) = \tfrac{1}{2}\left\{[E^C(k) + E^L] \pm \sqrt{[E^C(k) - E^L]^2 + 4V^2 \cdot x}\right\},$$

Broadening of subbands given by

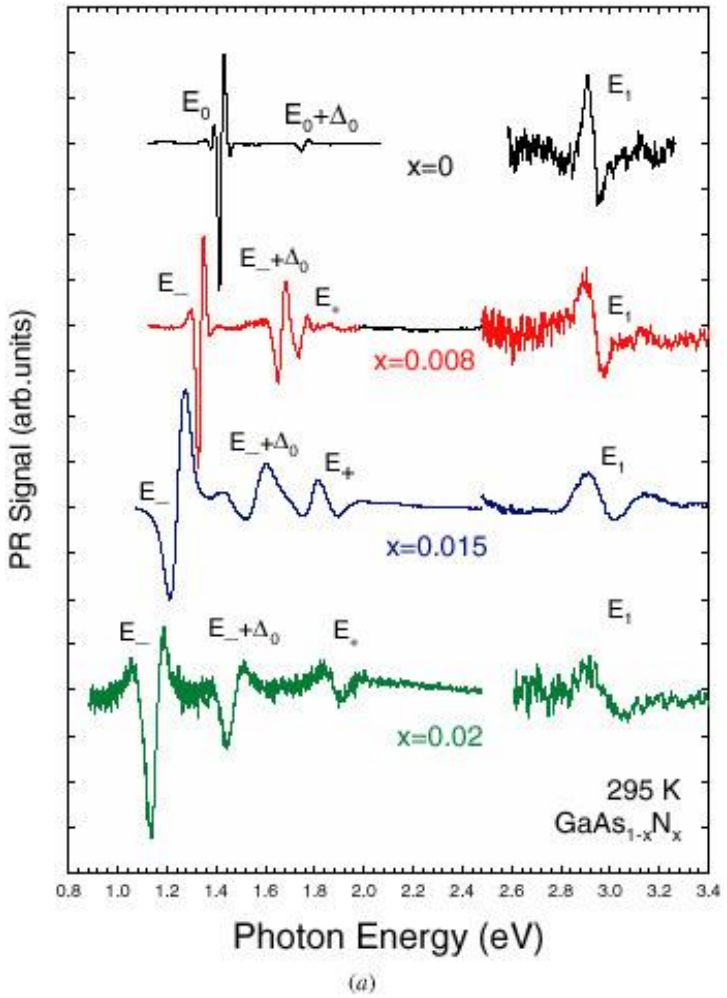
$$\Gamma_{\pm}(\mathbf{k}) = |\langle L | E_{\pm}(\mathbf{k})\rangle|^2 \cdot \Gamma_L.$$

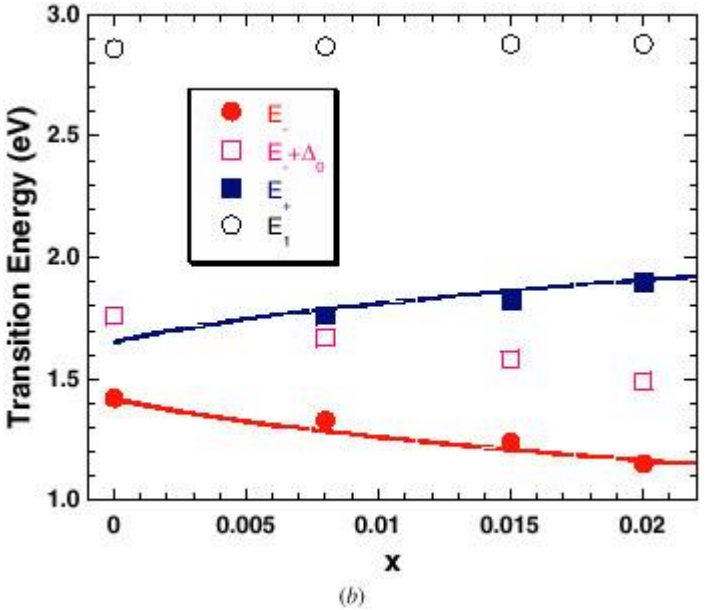
Comparison with Experiment – Energy gap reduction





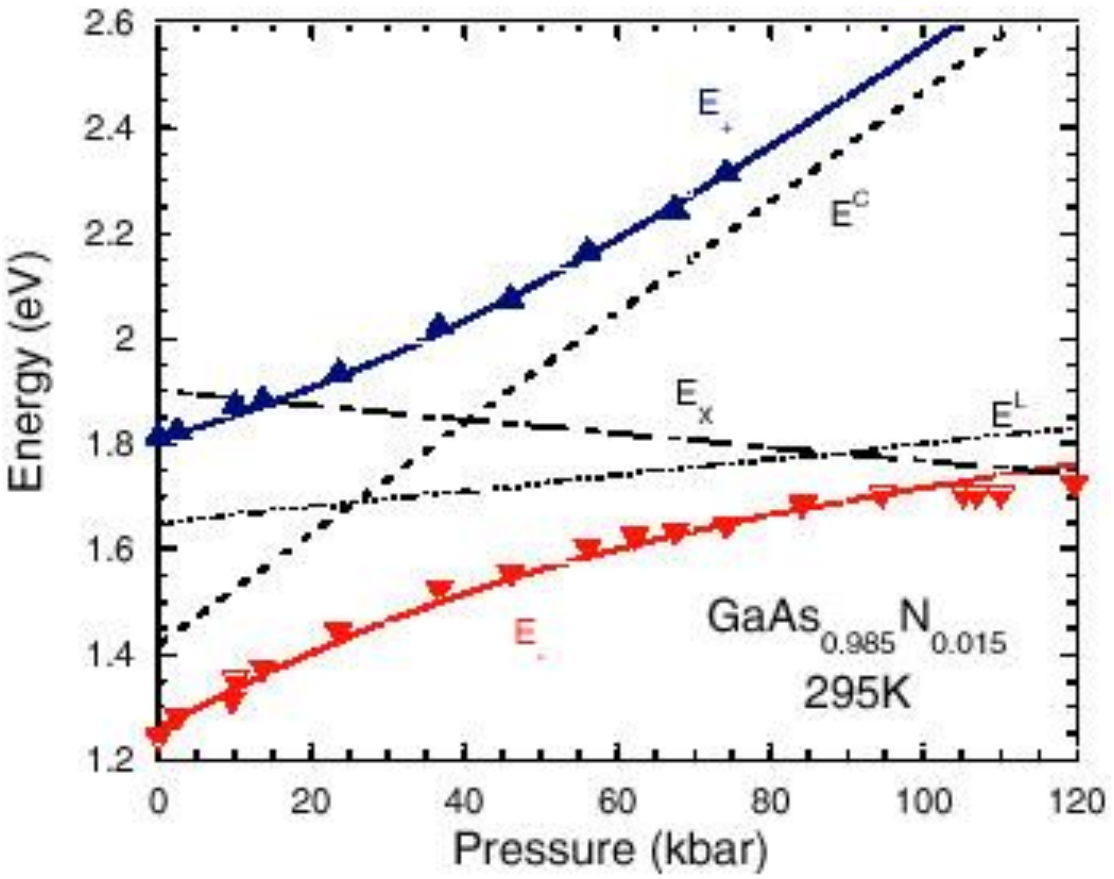
Comparison with Experiment – Photoreflectance spectroscopy





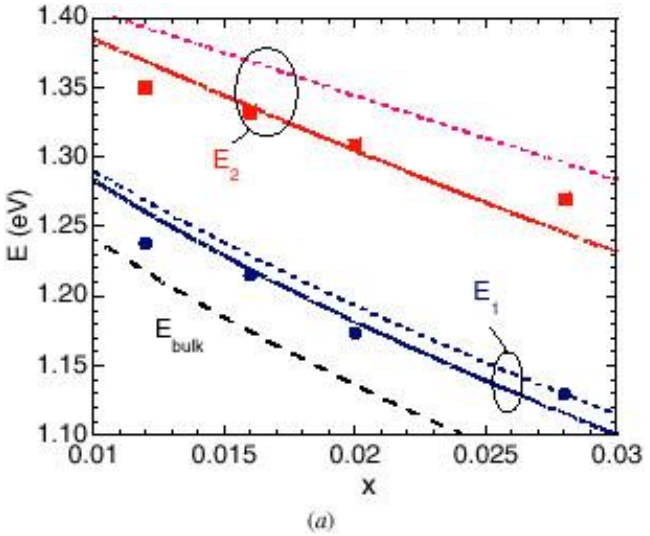
Away from the Brillouin zone center, the effect of substitutional N appears to be much weaker

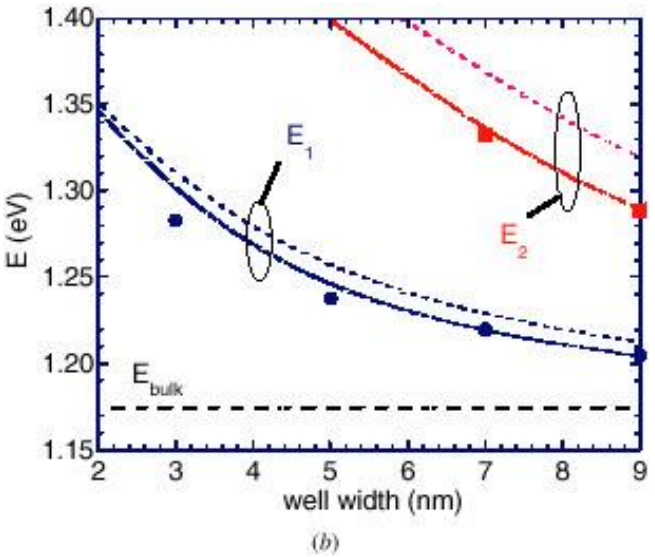
Comparison with Experiment – hydrostatic pressure



$$E_{\pm}(k) = \tfrac{1}{2}\left\{[E^{C}(k) + E^{L}] \pm \sqrt{[E^{C}(k) - E^{L}]^2 + 4V^2 \cdot x}\right\},$$

Band Anticrossing in QWs

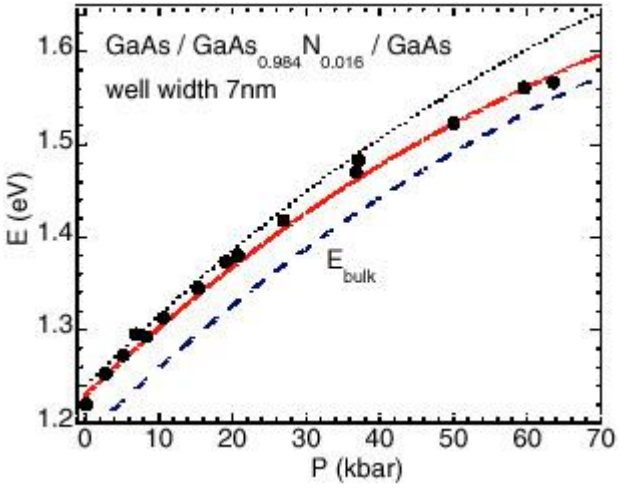




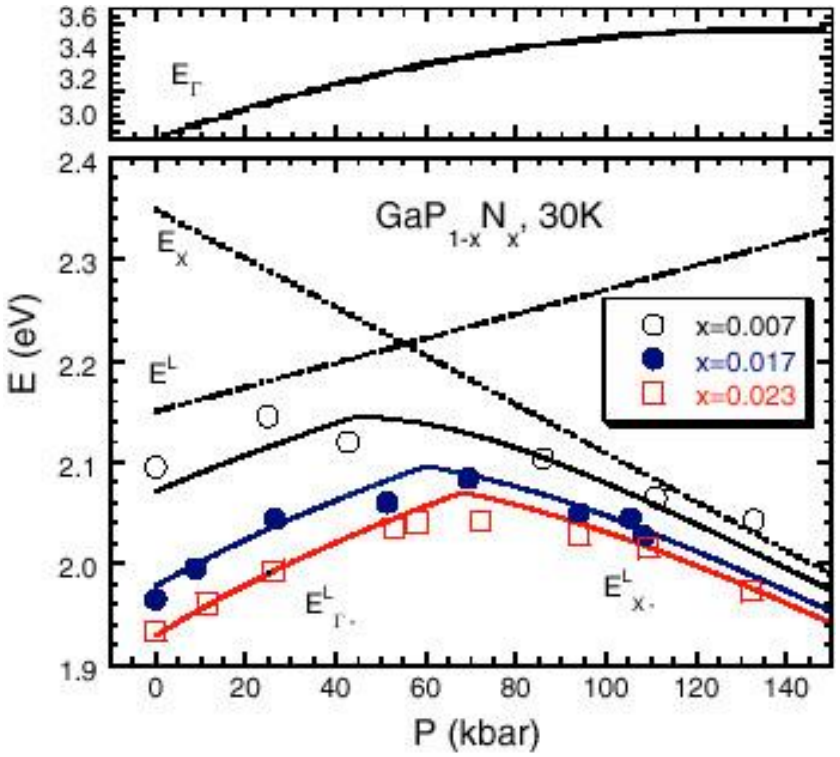
$$m^* \approx \hbar^2 \left| \frac{k}{\mathrm{d}E_-(k)/\mathrm{d}k} \right|_{k=0}$$

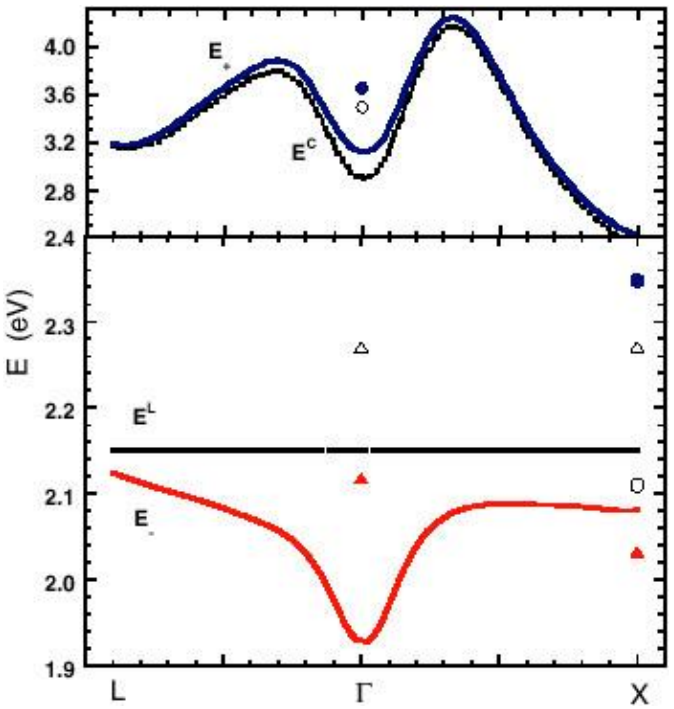
$$= 2m^*_{\mathrm{GaAs}} \Bigg/ \left[1 - \frac{E^C(0) - E^L}{\sqrt{(E^C(0) - E^L)^2 + 4V^2x}} \right].$$

Effective mass adjustment from the BAC

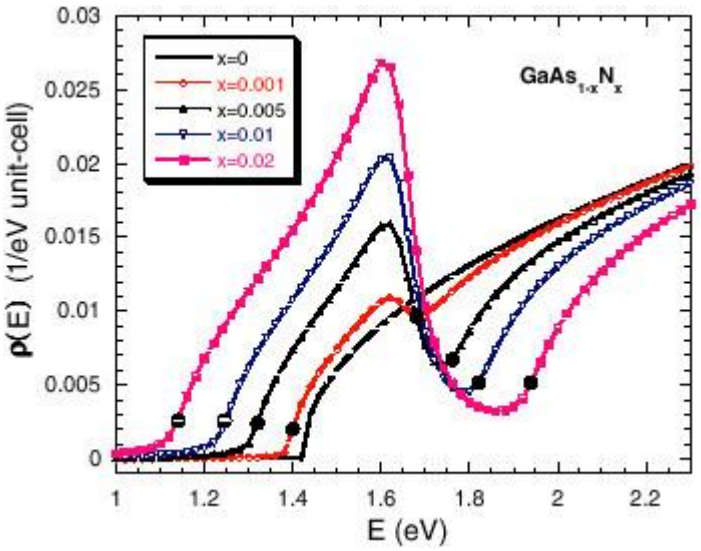


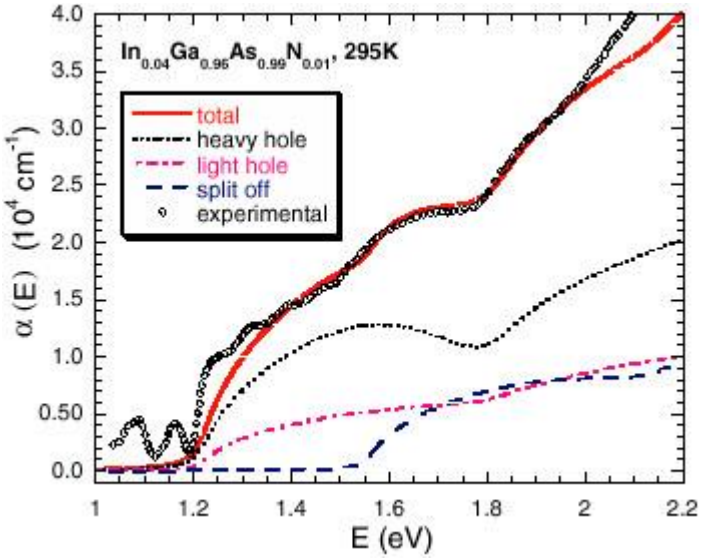
Band Anticrossing in the entire Brillouin zone





State broadening



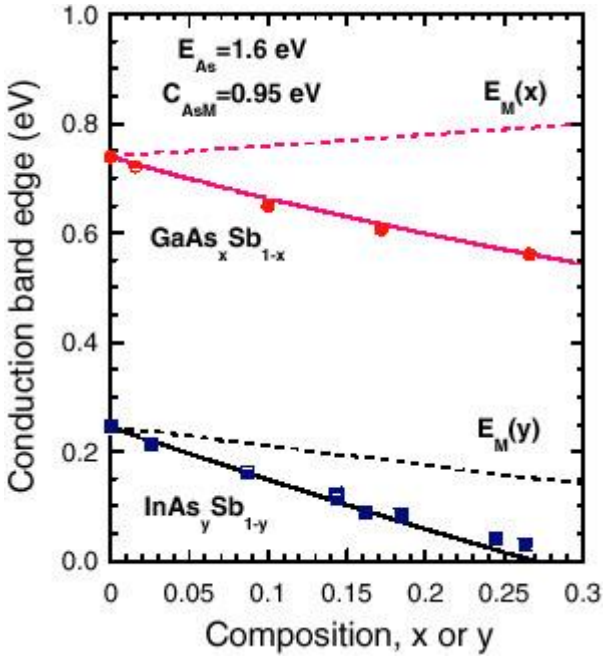


State broadening on optical properties

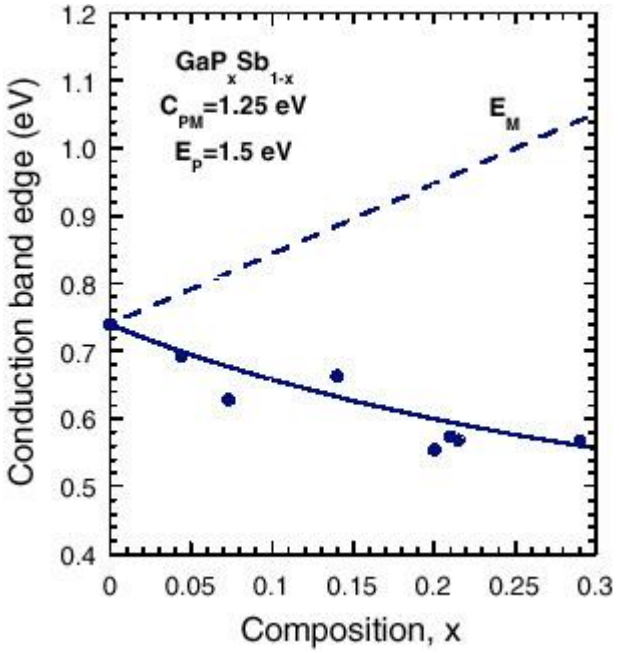
- Density of states for GaAs
- Perturbed density of states

BAC in other alloys

Some other of the III-V and II-VI alloys have anions with a small but still significant difference in electronegativity



BAC effects are small in GaAsSb and InAsSb because Sb and As only differ slightly in electronegativity ($\Delta = 0.2$)



Larger effects where P replaces Sb ($\Delta = 0.3$)

For example, N and As ($\Delta = 0.86$)

Thank You

Questions?