EE-612:
Lecture 31:
Heterostructure Fundamentals

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NCN

www.nanohub.org

PURDUE UNIVERSITY

outline

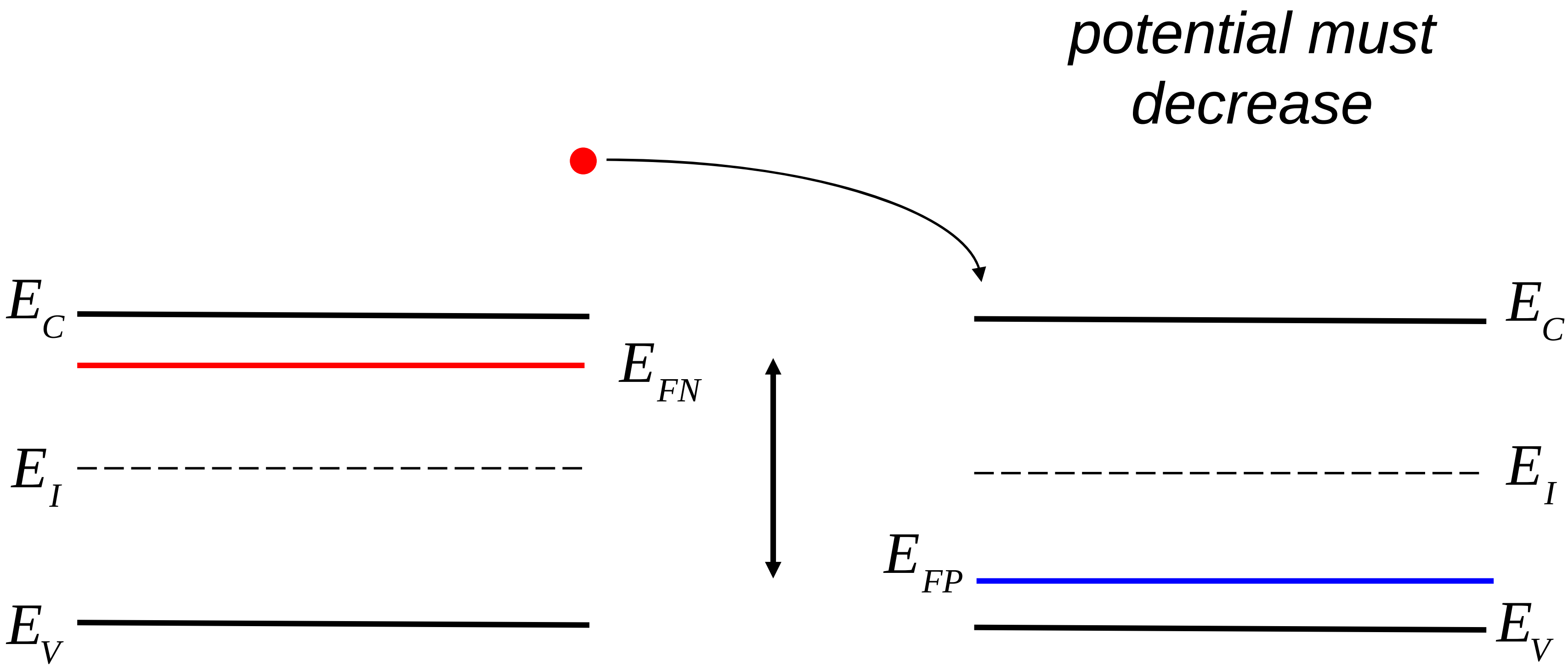
1. **Introduction**
2. Energy bands in abrupt heterojunctions
3. Depletion approximation
4. Poisson-Boltzmann equation
5. Energy bands in graded heterojunctions
6. Drift-diffusion equation for heterostructures
7. Heavy doping effects and heterostructures
8. Band offsets

reference

This presentation is based on a set of notes, which contains detailed derivations of the results presented here.

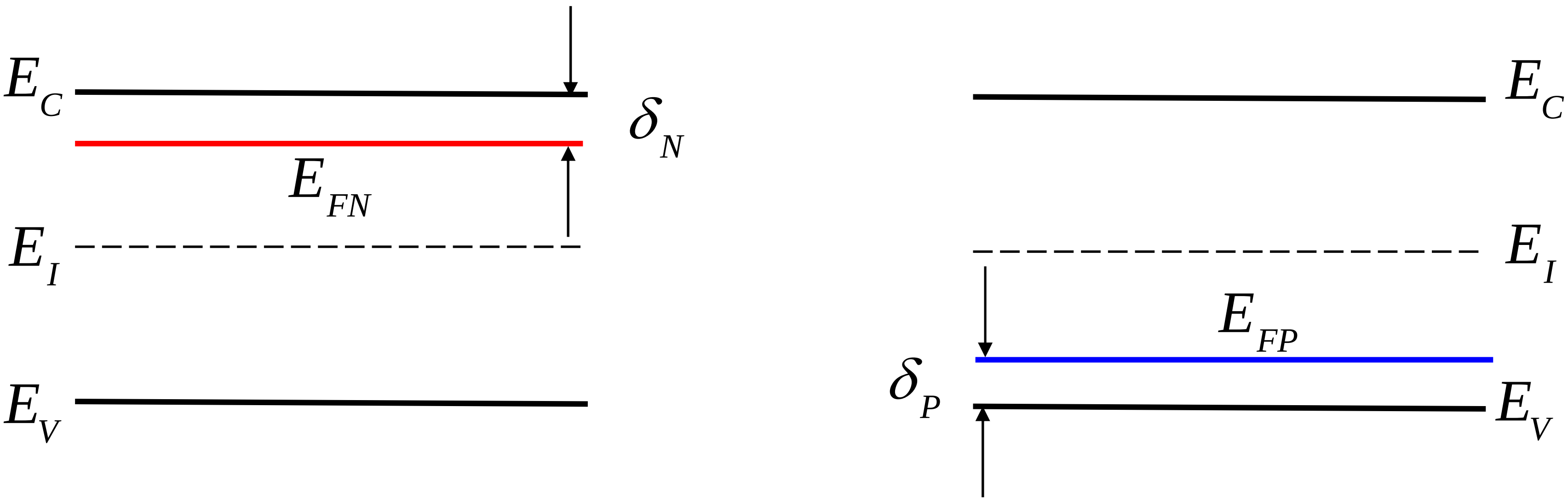
"Heterostructure Fundamentals," by Mark Lundstrom, Purdue University, Fall, 1995.

review: pn homojunctions



$$qV_{BI} = \left(E_{FN} - E_{FP}\right)/q$$

built-in potential



$$qV_{BI} = \left(E_{FN} - E_{FP}\right)$$

$$N_D = N_C e^{-\delta_N / k_B T}$$

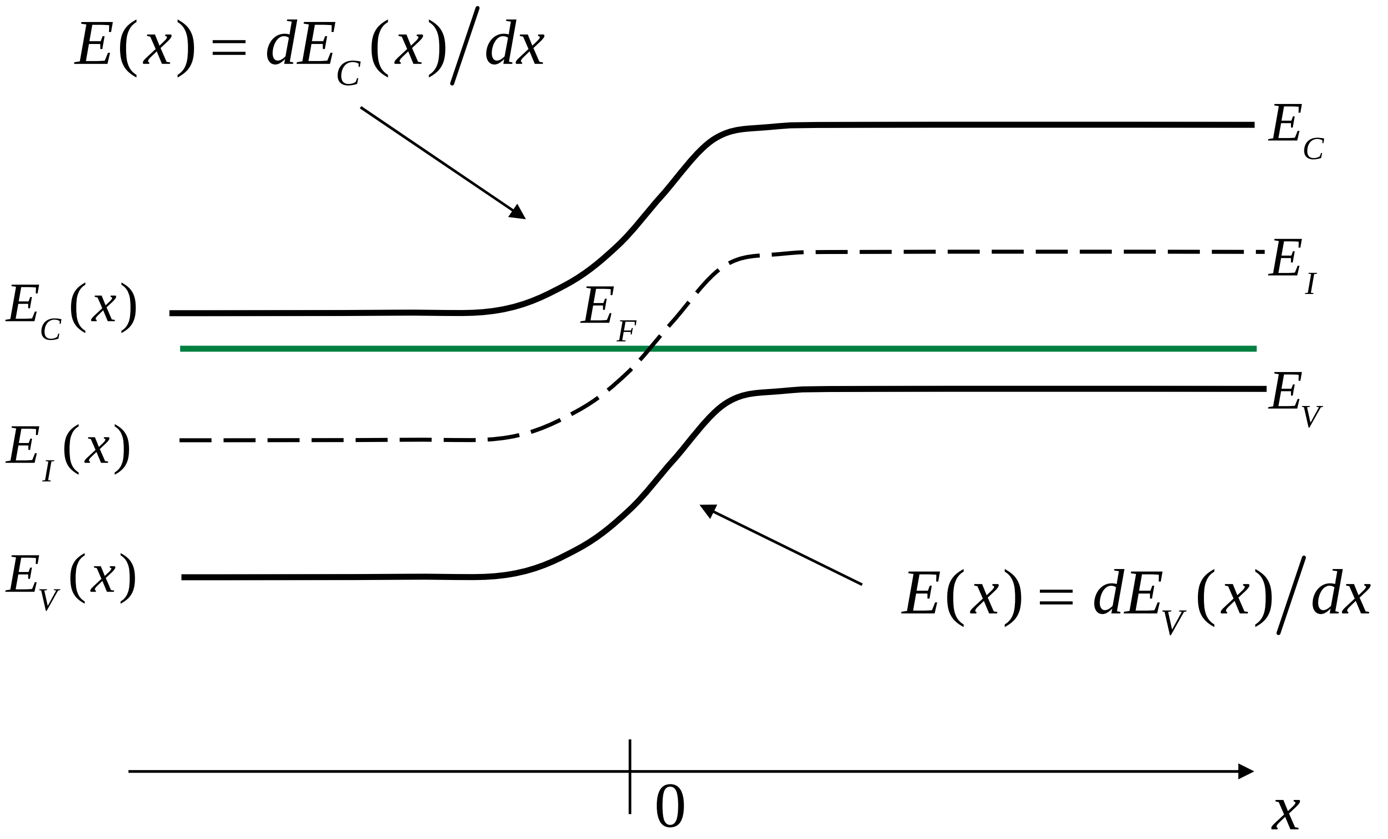
$$qV_{BI} = \left(E_C - E_V\right) - \delta_N - \delta_P$$

$$N_A = N_V e^{-\delta_P / k_B T}$$

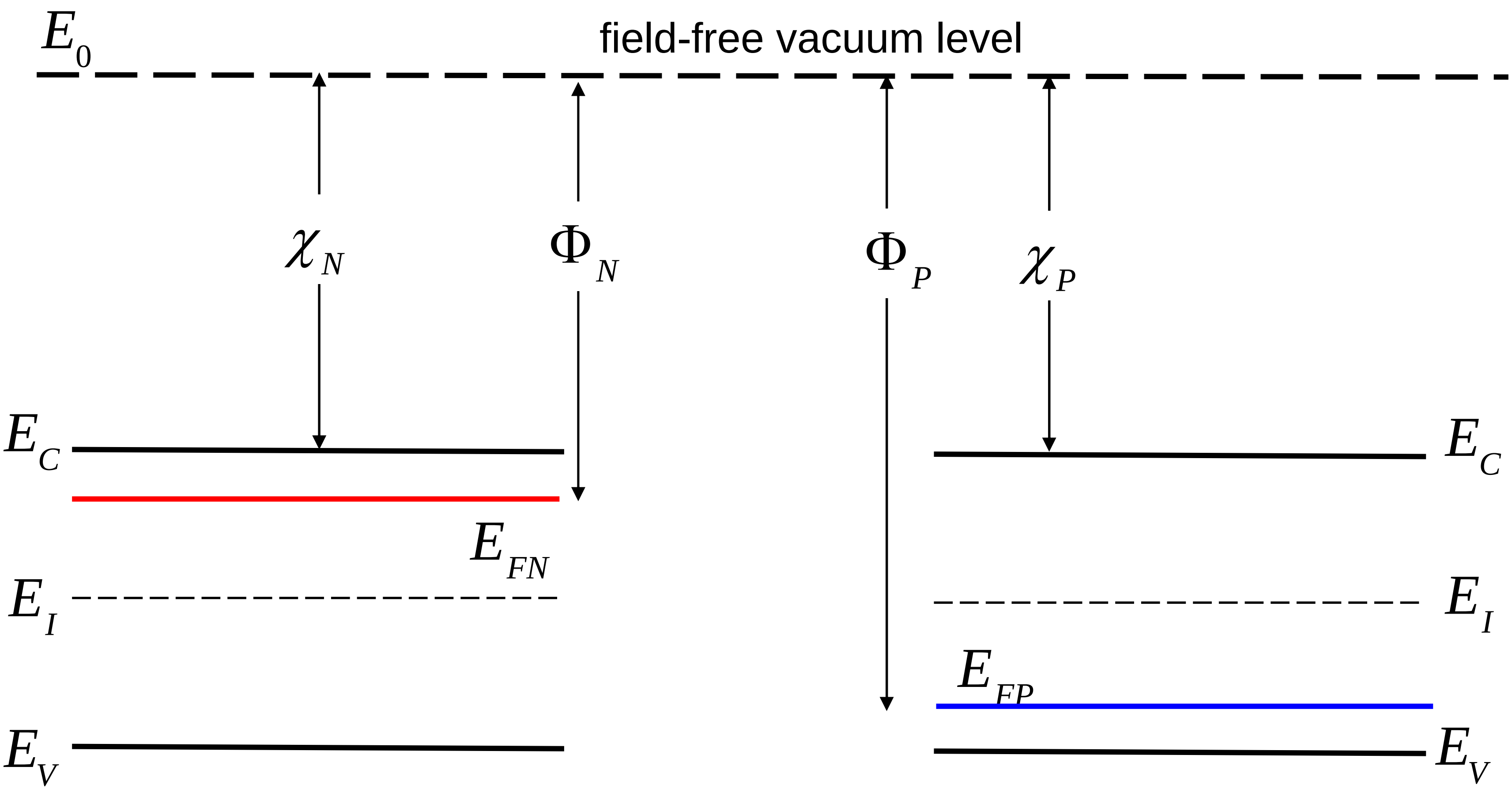
$$qV_{BI} = E_G - \delta_N - \delta_P$$

$$qV_{BI} = k_B T \ln\left(N_A N_D / n_i^2\right)$$

review: pn homojunctions



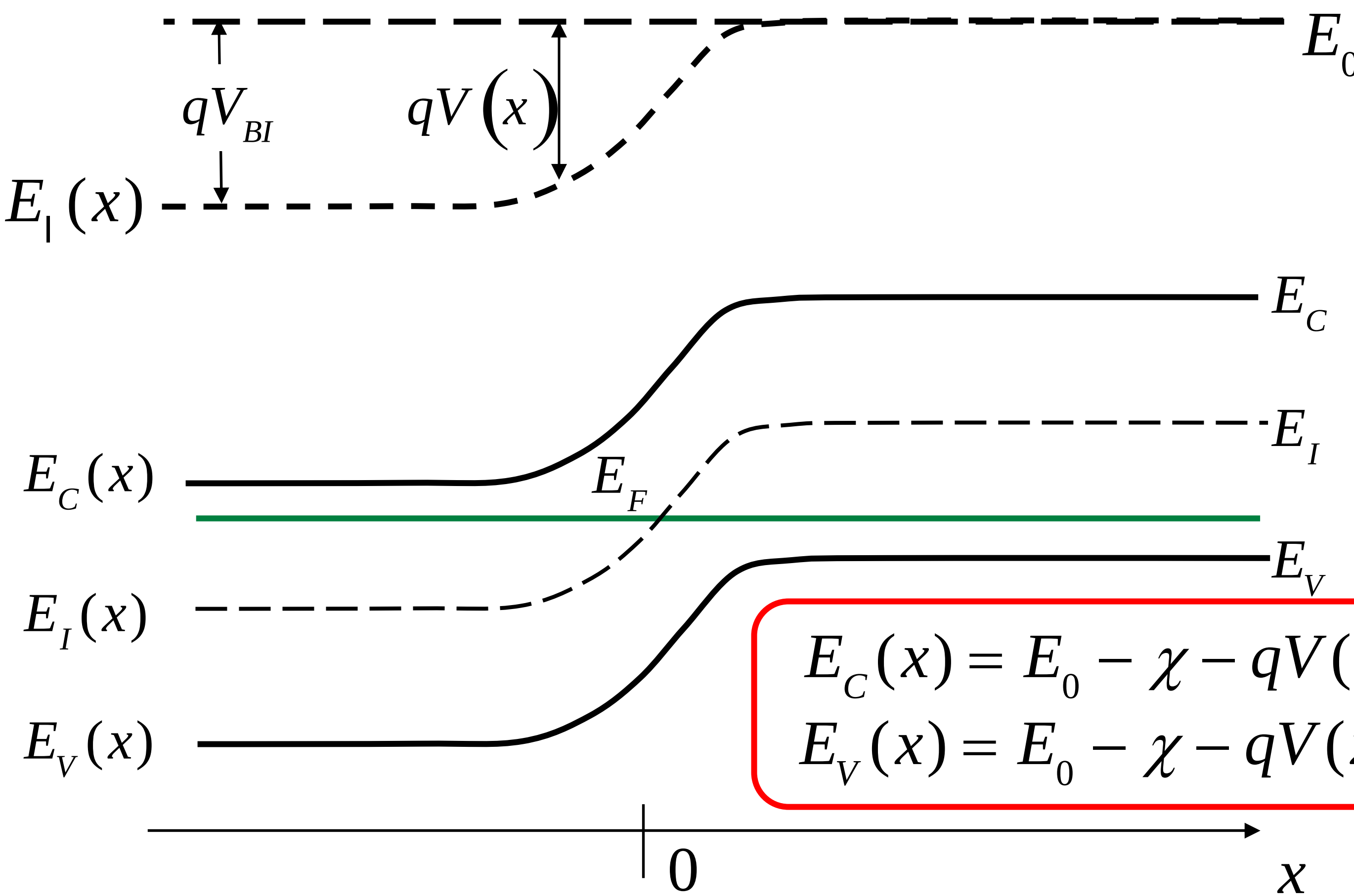
reference for the energy bands



$$E_C = E_0 - \chi$$
$$E_V = E_0 - \chi - E_G$$

$$qV_{BI} = \left(\Phi_P - \Phi_N\right)$$

local vacuum level



$$E_C(x) = E_0 - \chi - qV(x)$$

$$E_V(x) = E_0 - \chi - qV(x) - E_G$$

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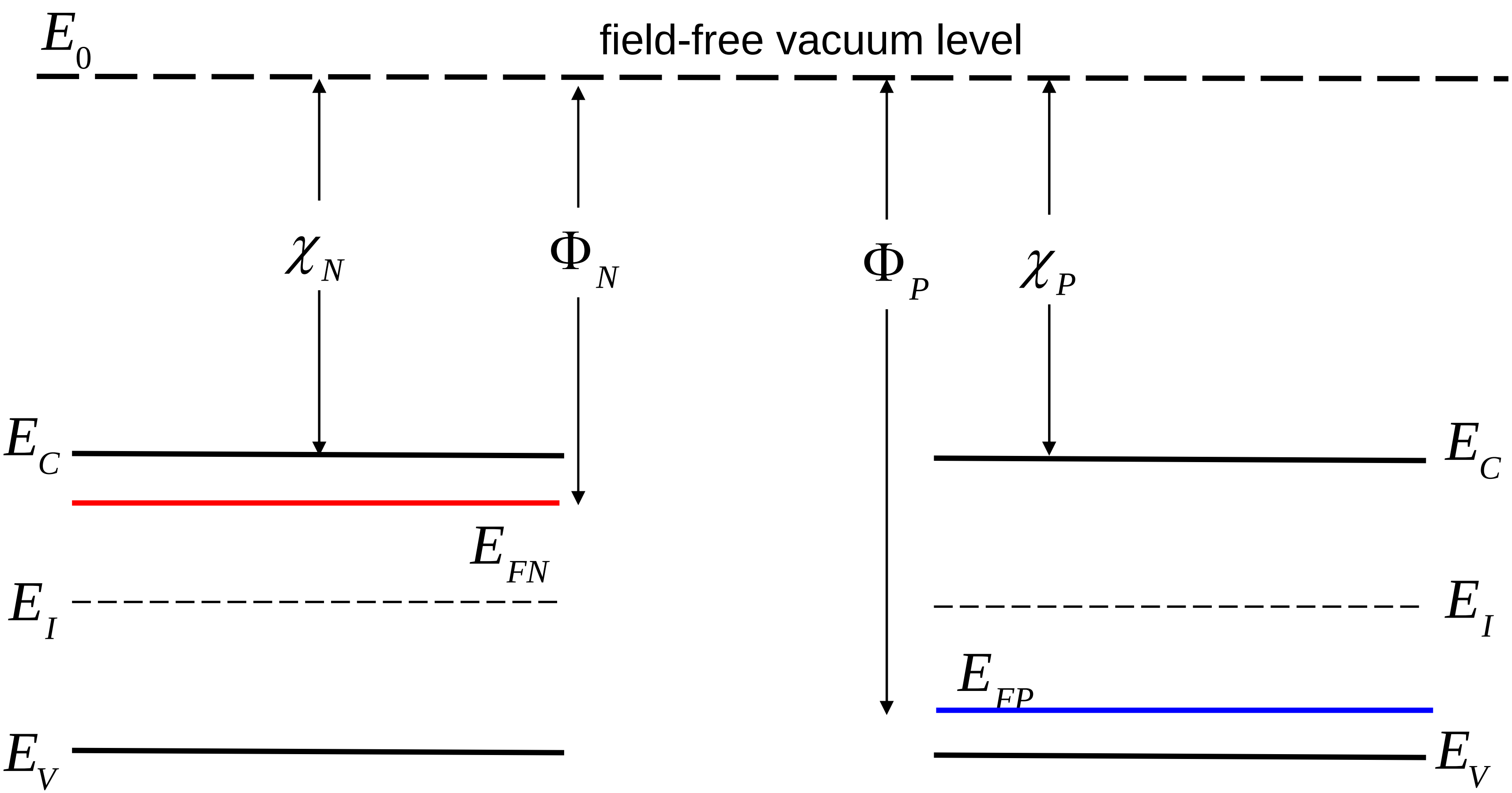
reference for the energy bands

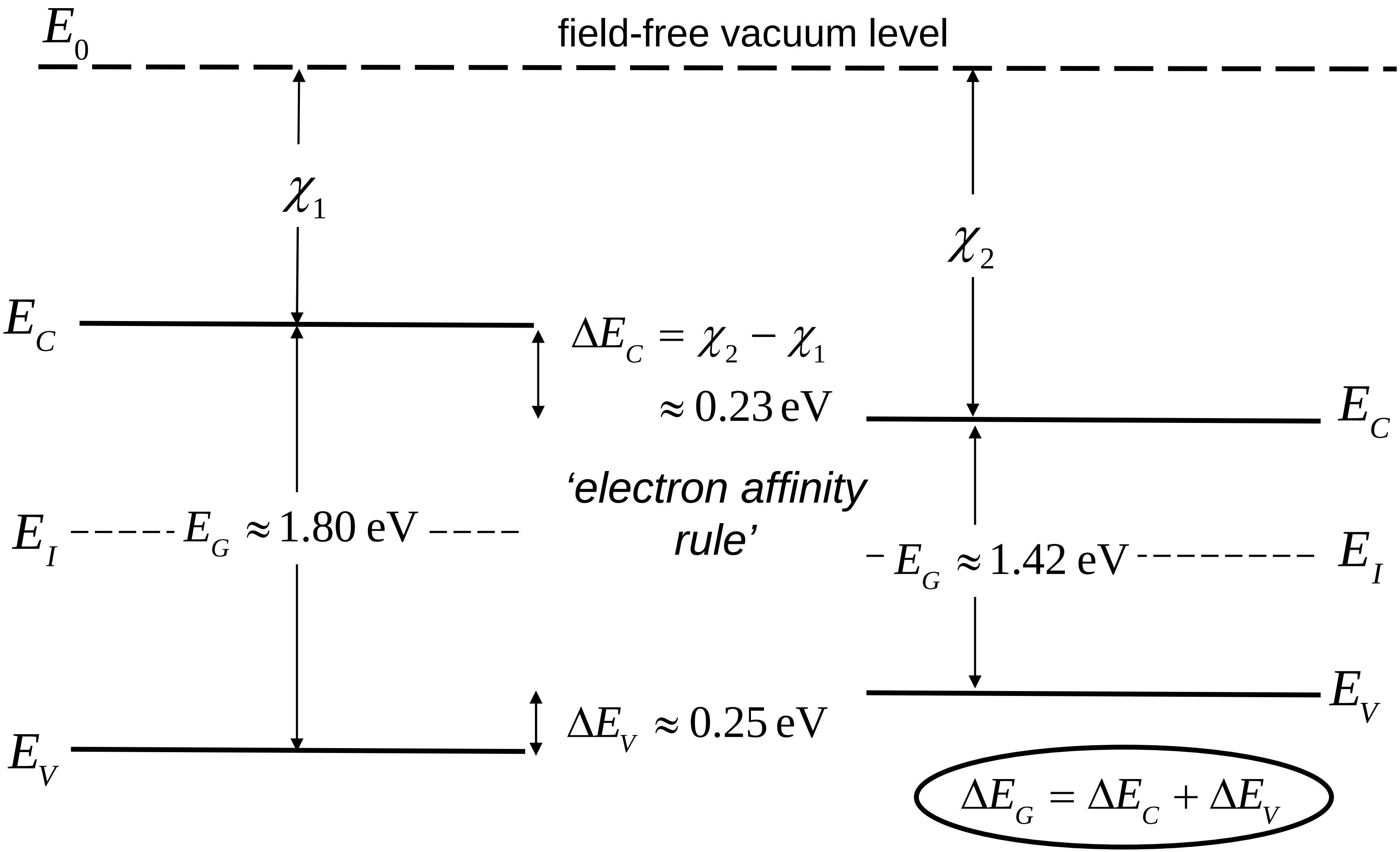


$$E_C = E_0 - \chi$$

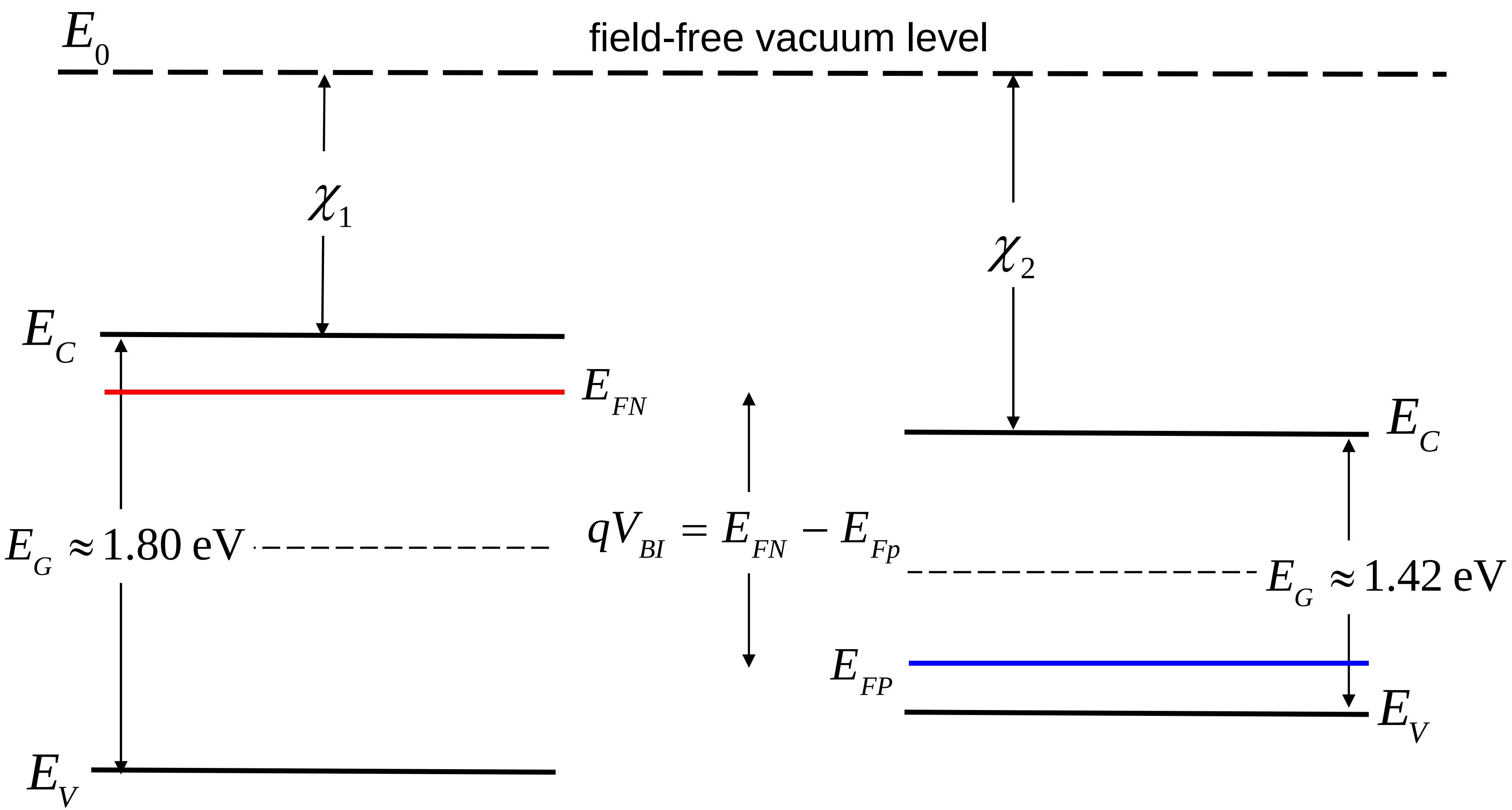
$$E_V = E_0 - \chi - E_G$$

$$qV_{BI} = \left(\Phi_P - \Phi_N\right)$$

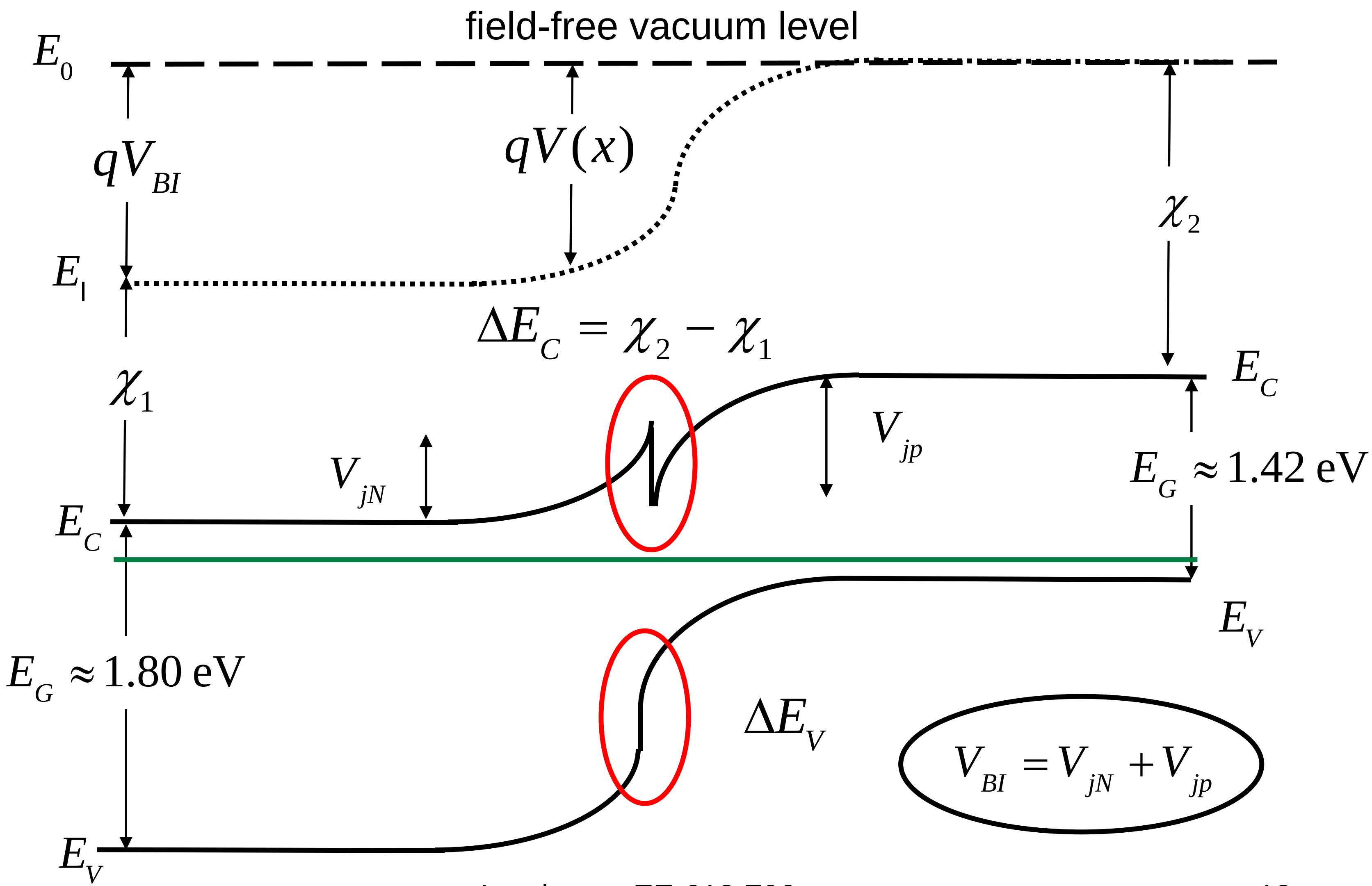
$Al_{0.3}Ga_{0.7}As$: GaAs (Type I HJ)



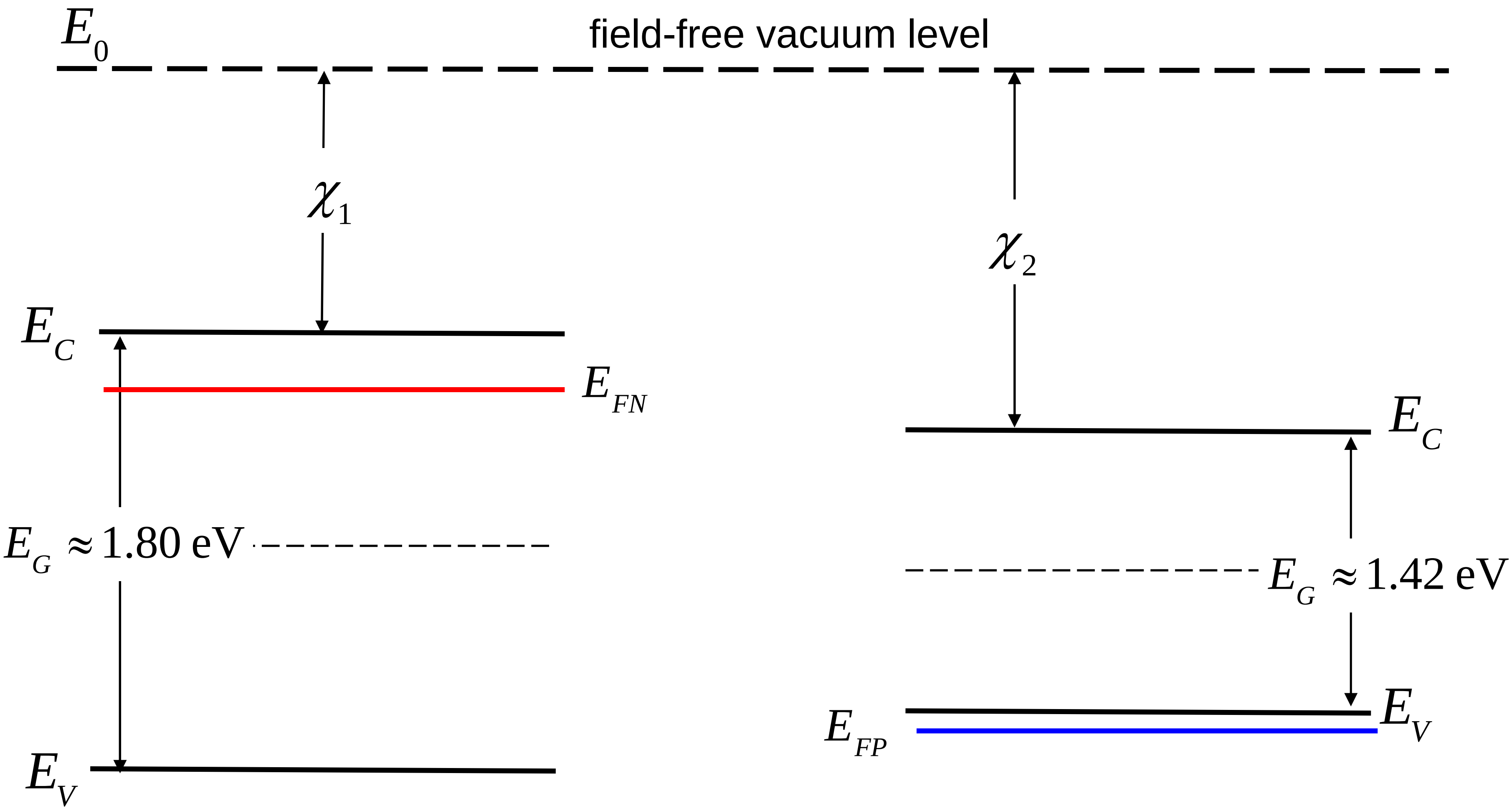
N-$Al_{0.3}Ga_{0.7}As$: p-GaAs (Type I HJ)



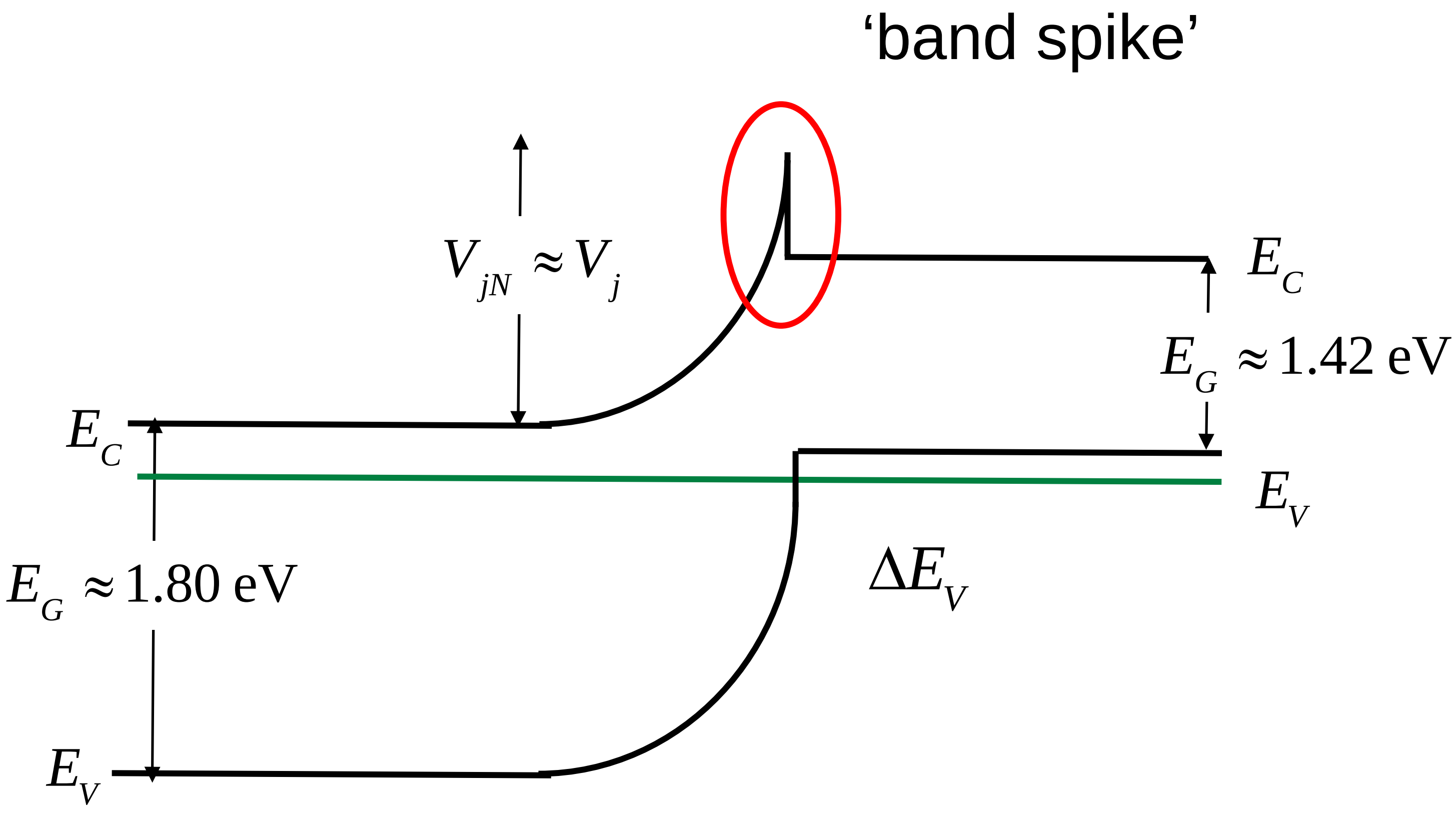
N-$Al_{0.3}Ga_{0.7}As$: p-GaAs (Type I HJ)



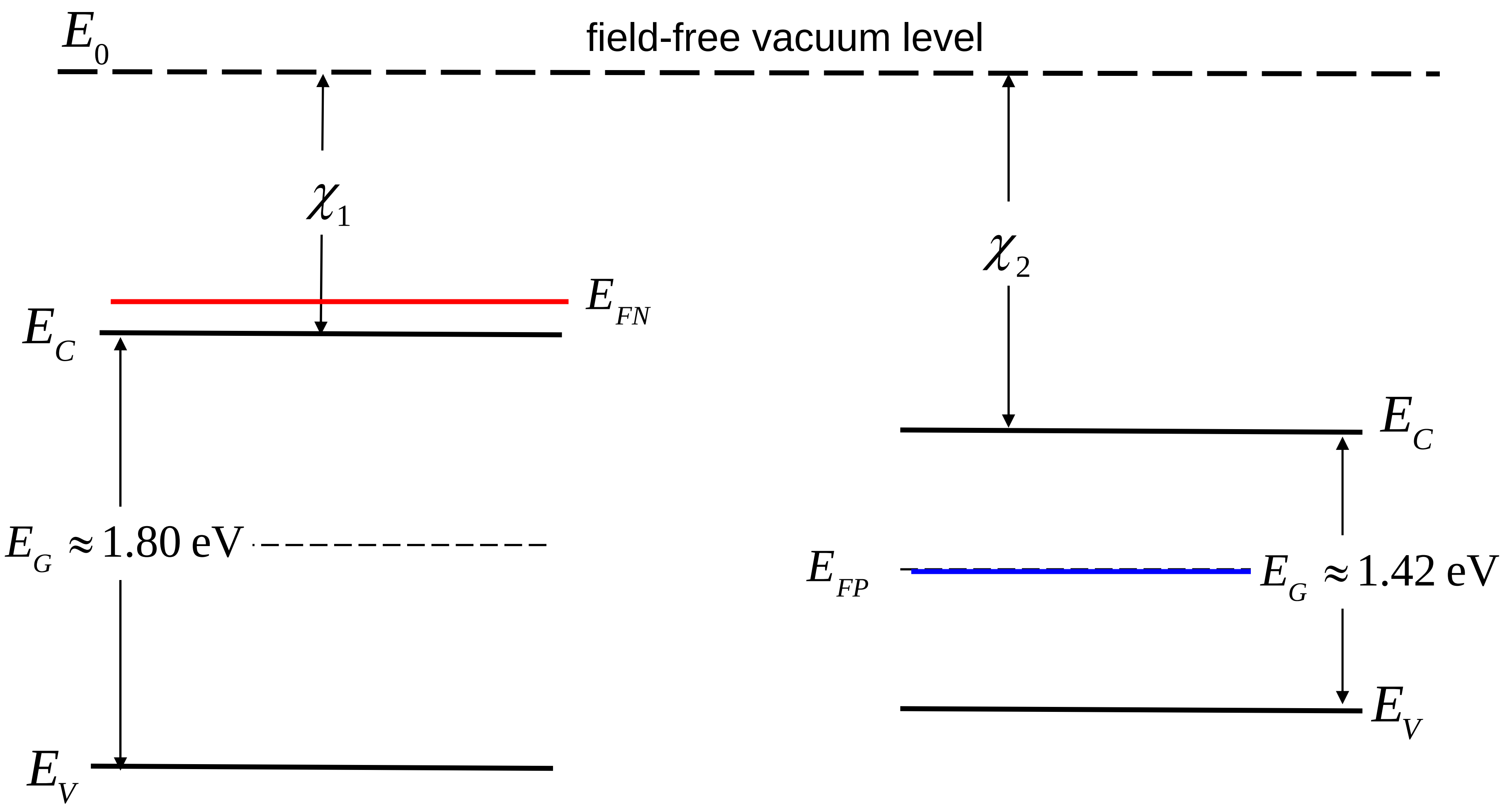
N-$Al_{0.3}Ga_{0.7}As$: p^+-GaAs



N-$Al_{0.3}Ga_{0.7}As$: p-GaAs



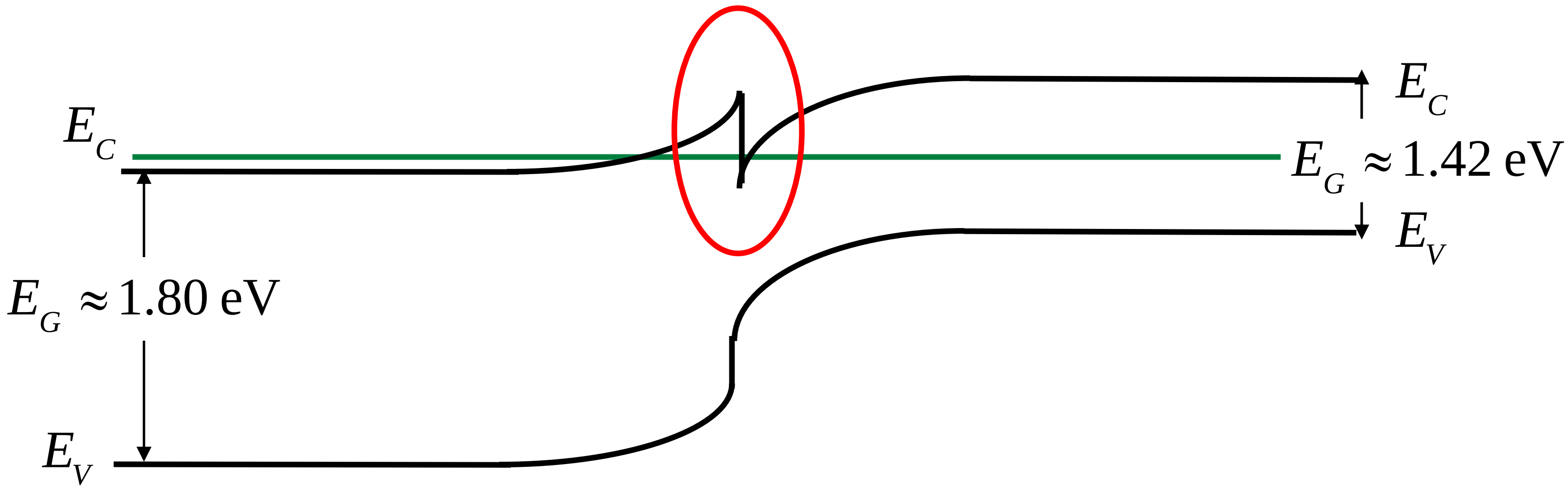
N^+-$Al_{0.3}Ga_{0.7}As$: i-GaAs



N-$Al_{0.3}Ga_{0.7}As$: i-GaAs

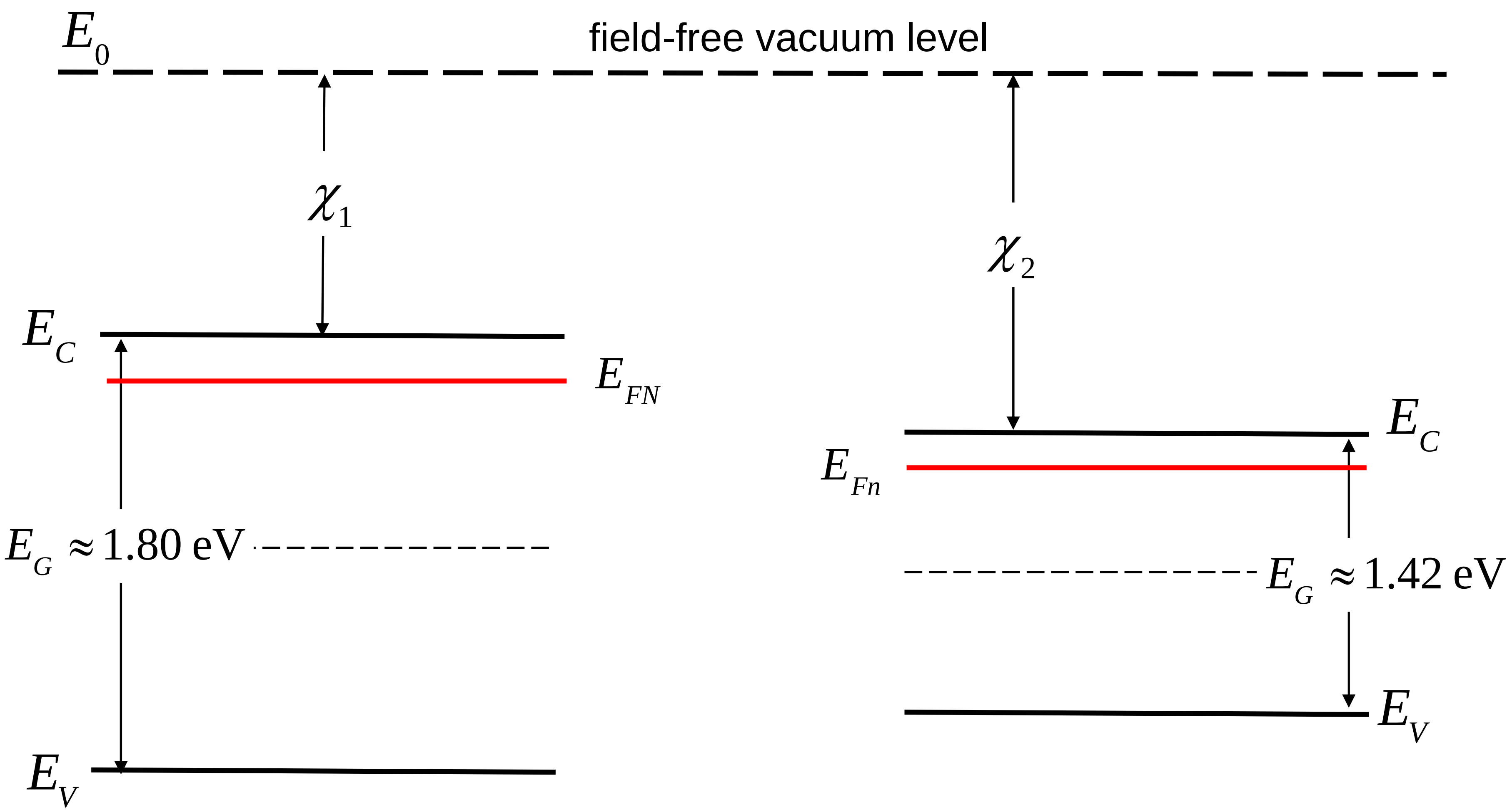
‘modulation doping’

‘2D electron gas’



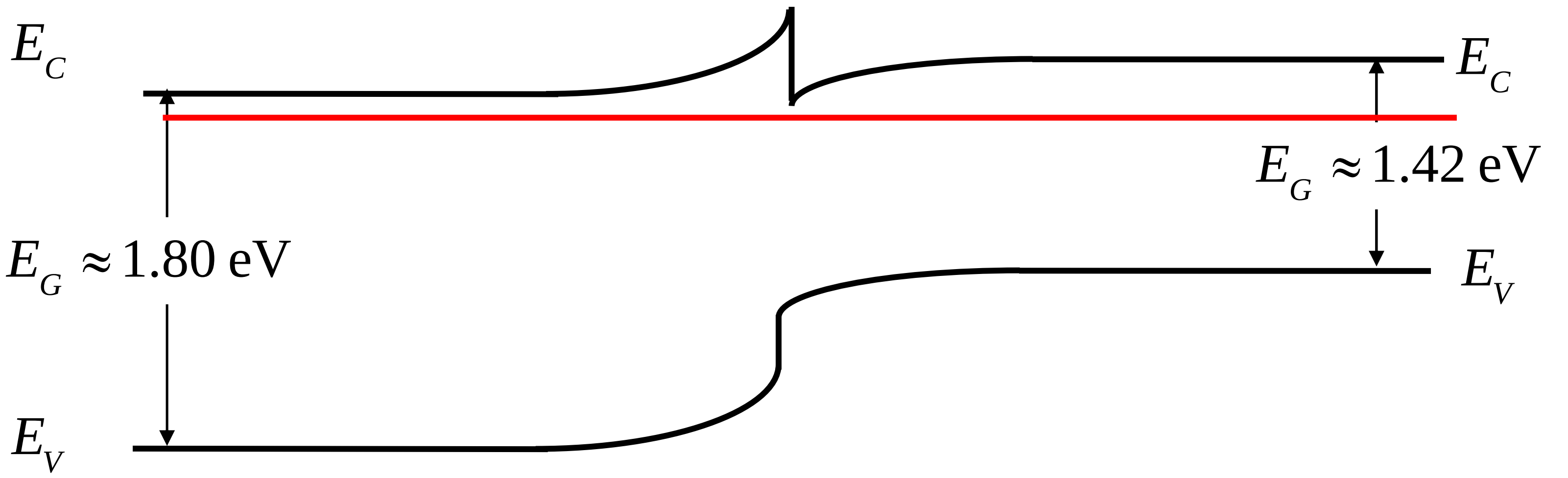
depletion layer inversion/accumulation layer

N-$Al_{0.3}Ga_{0.7}As$: n-GaAs



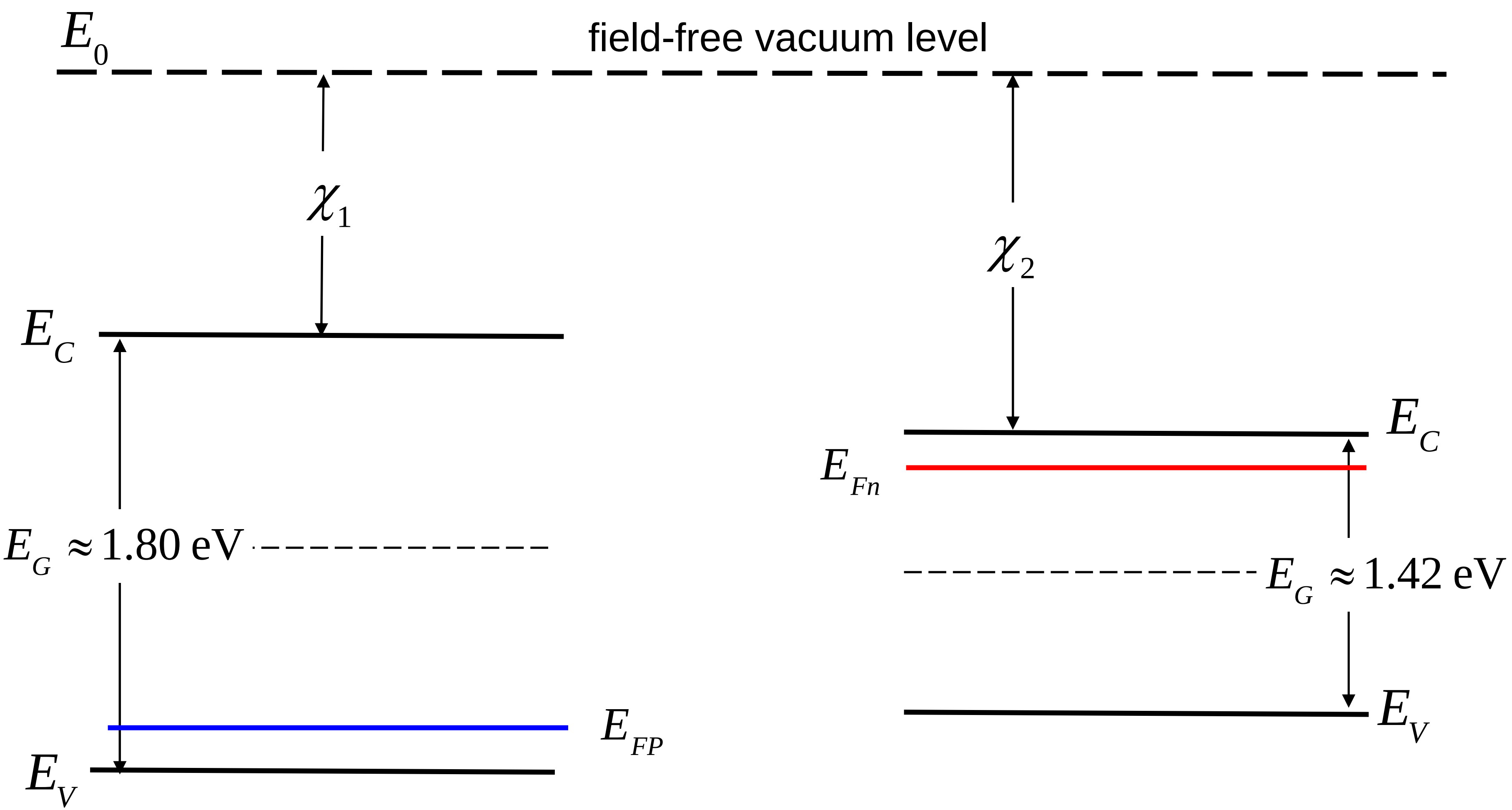
N-$Al_{0.3}Ga_{0.7}As$: i-GaAs

'isotype heterojunction'

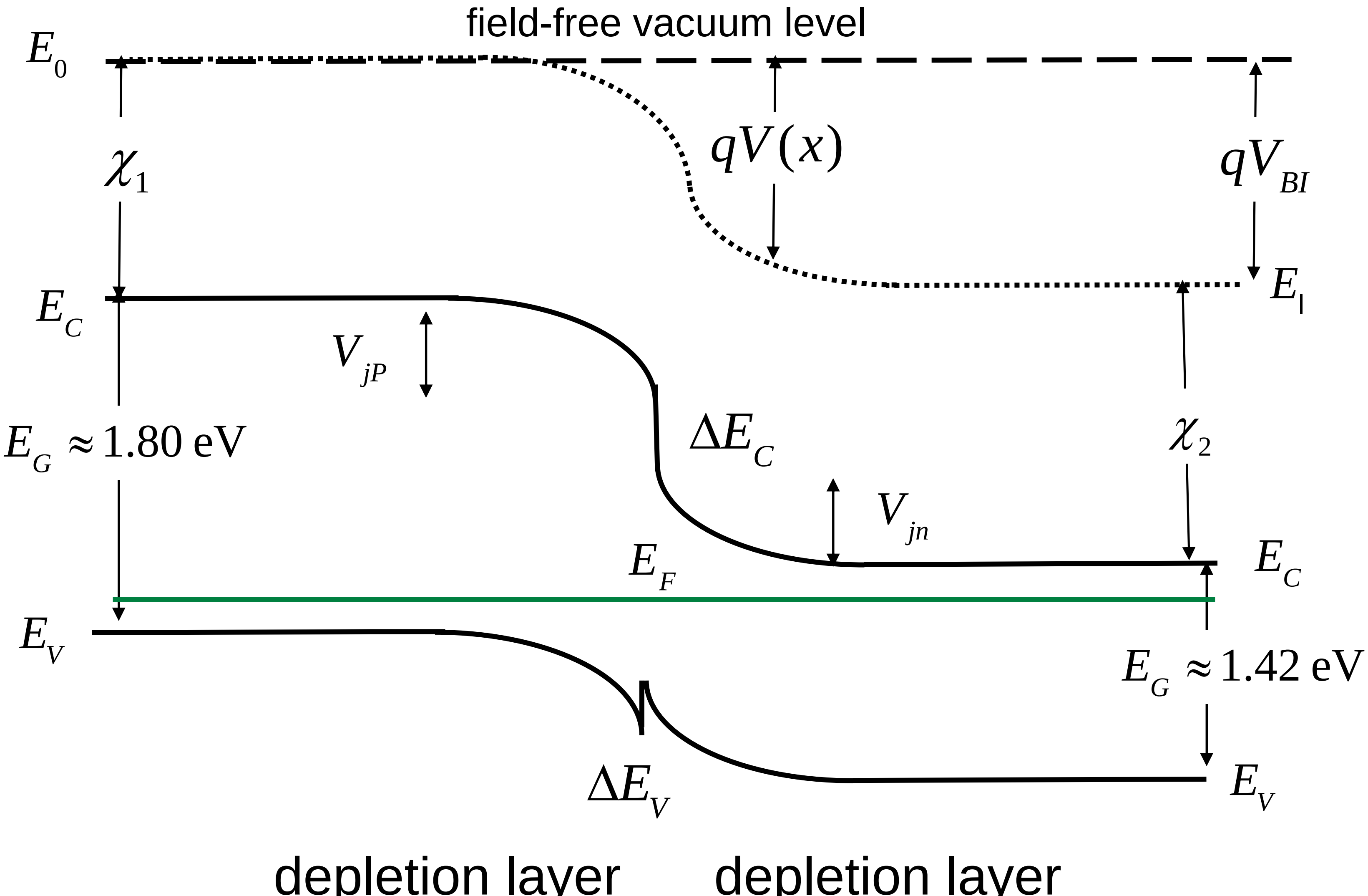


depletion layer accumulation layer

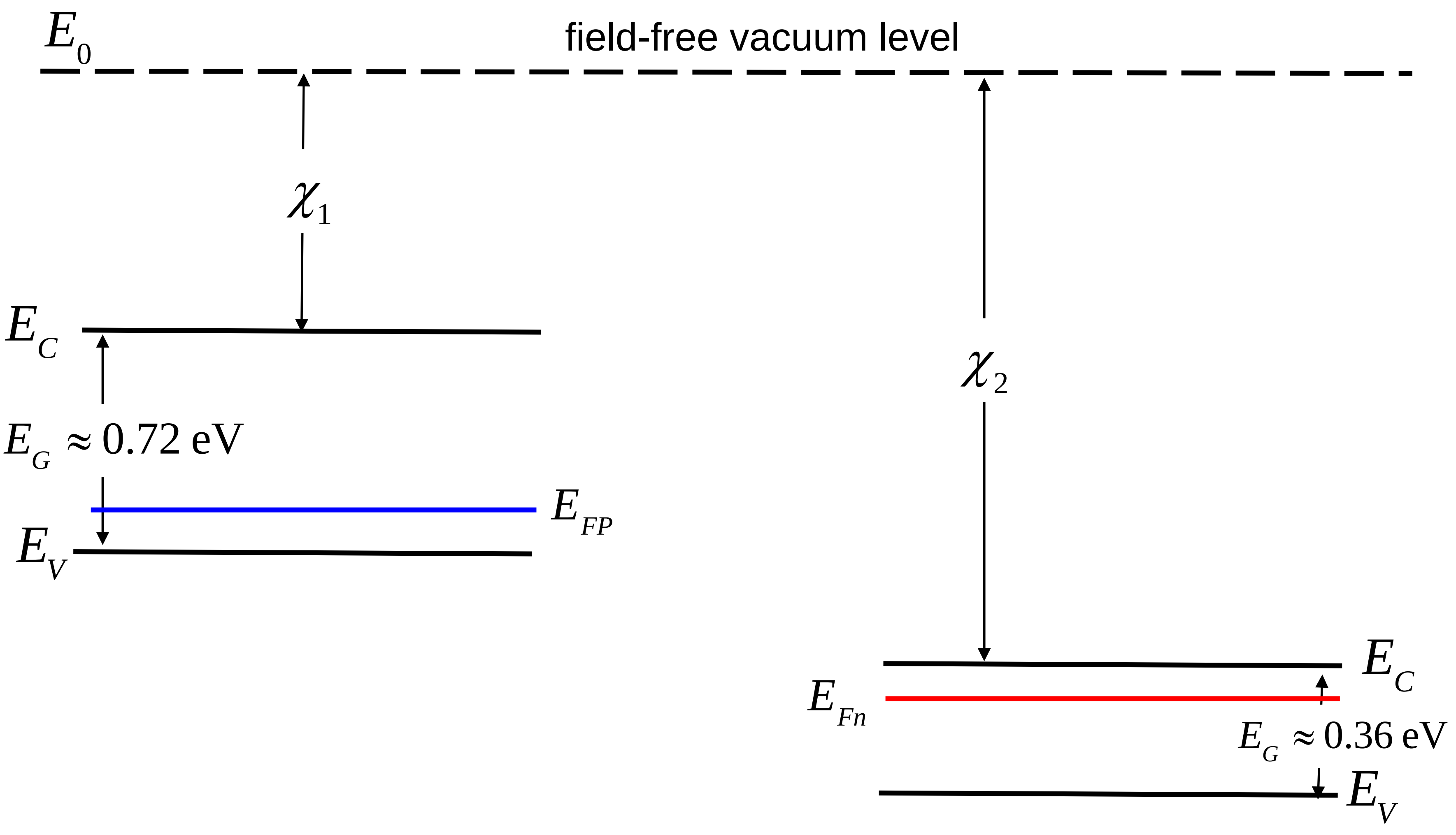
P-$Al_{0.3}Ga_{0.7}As$: n-GaAs



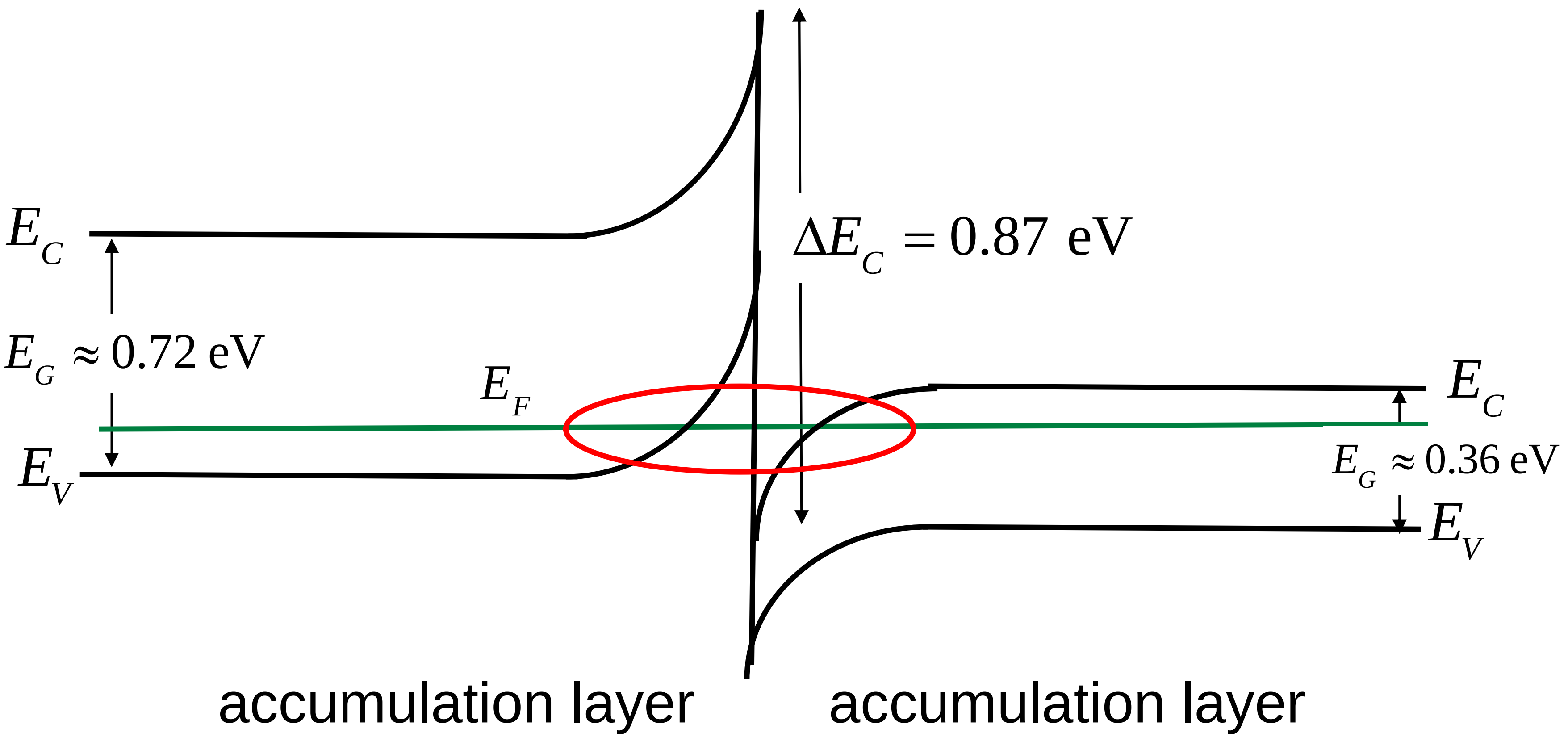
P-$Al_{0.3}Ga_{0.7}As$: n-GaAs



P-GaSb : n-InAs (Type III)



P-GaSb : n-InAs (Type III)



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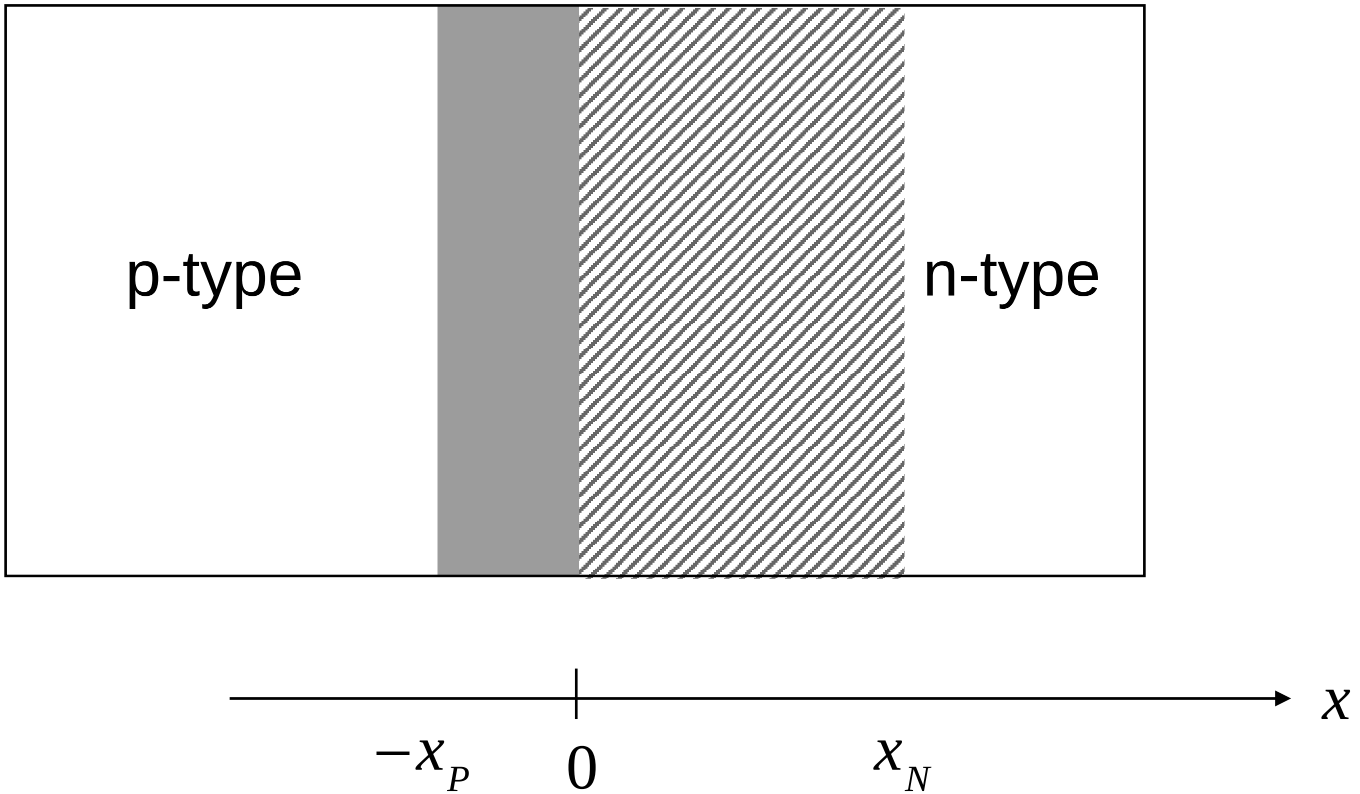
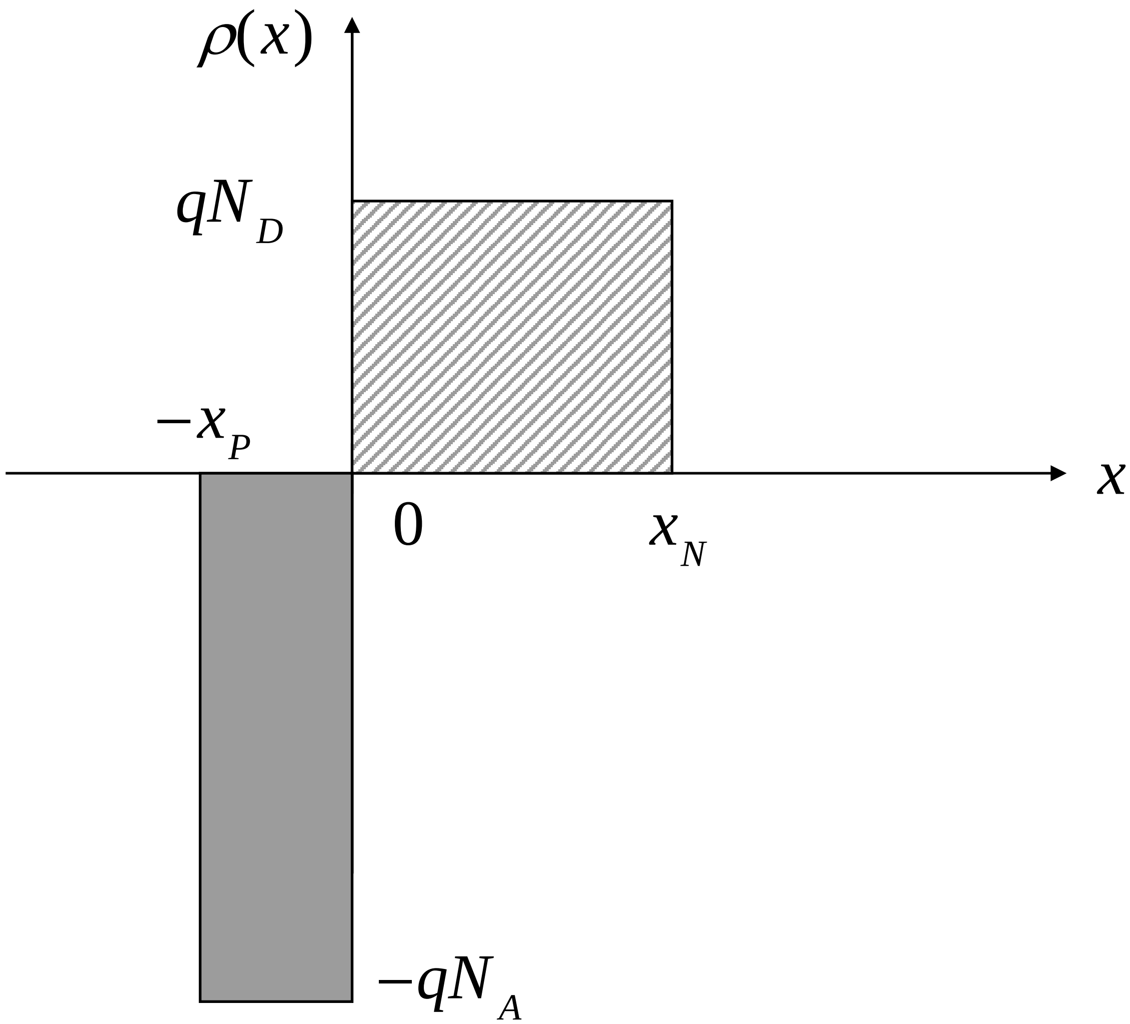
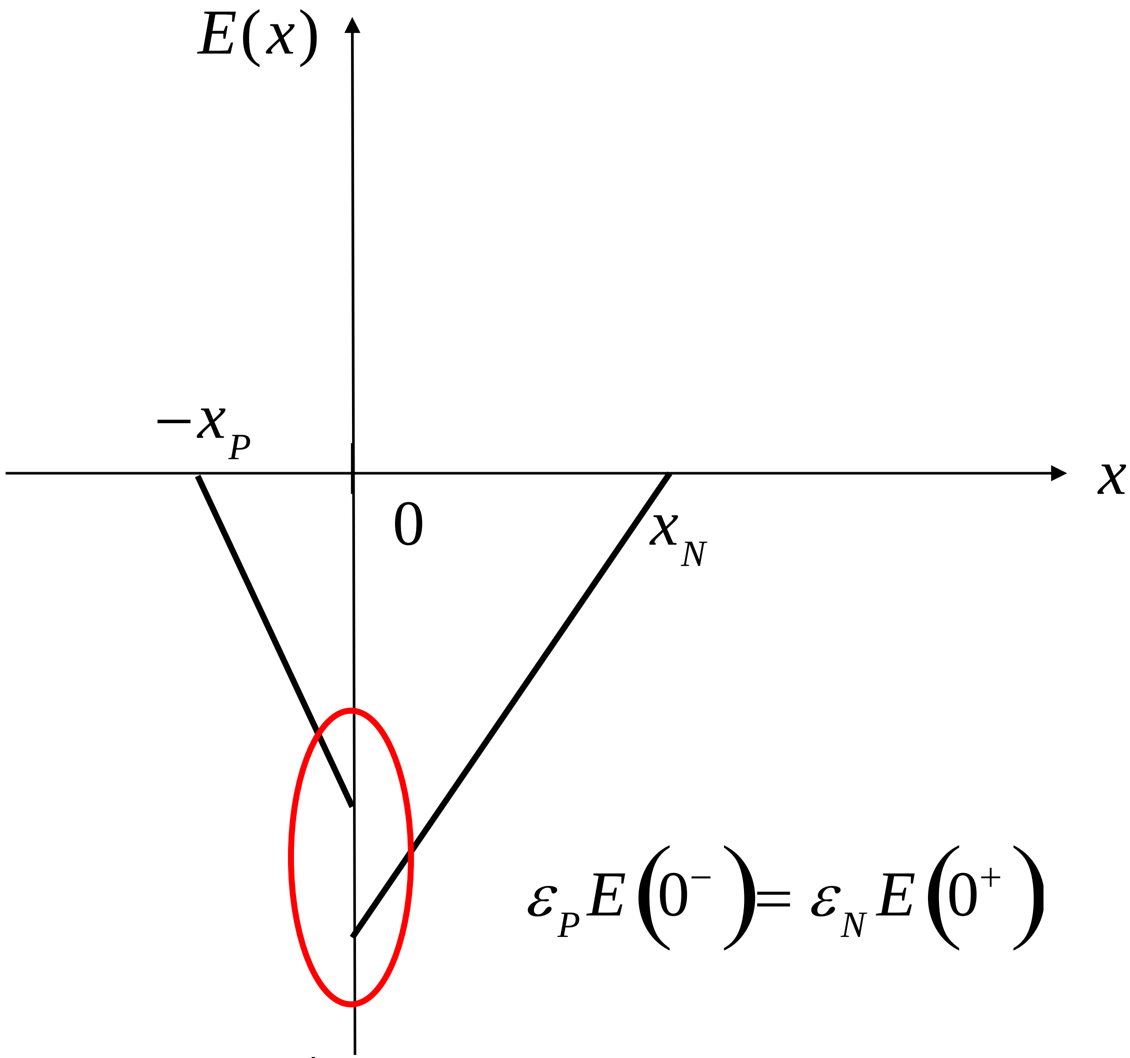
geometry



space charge density

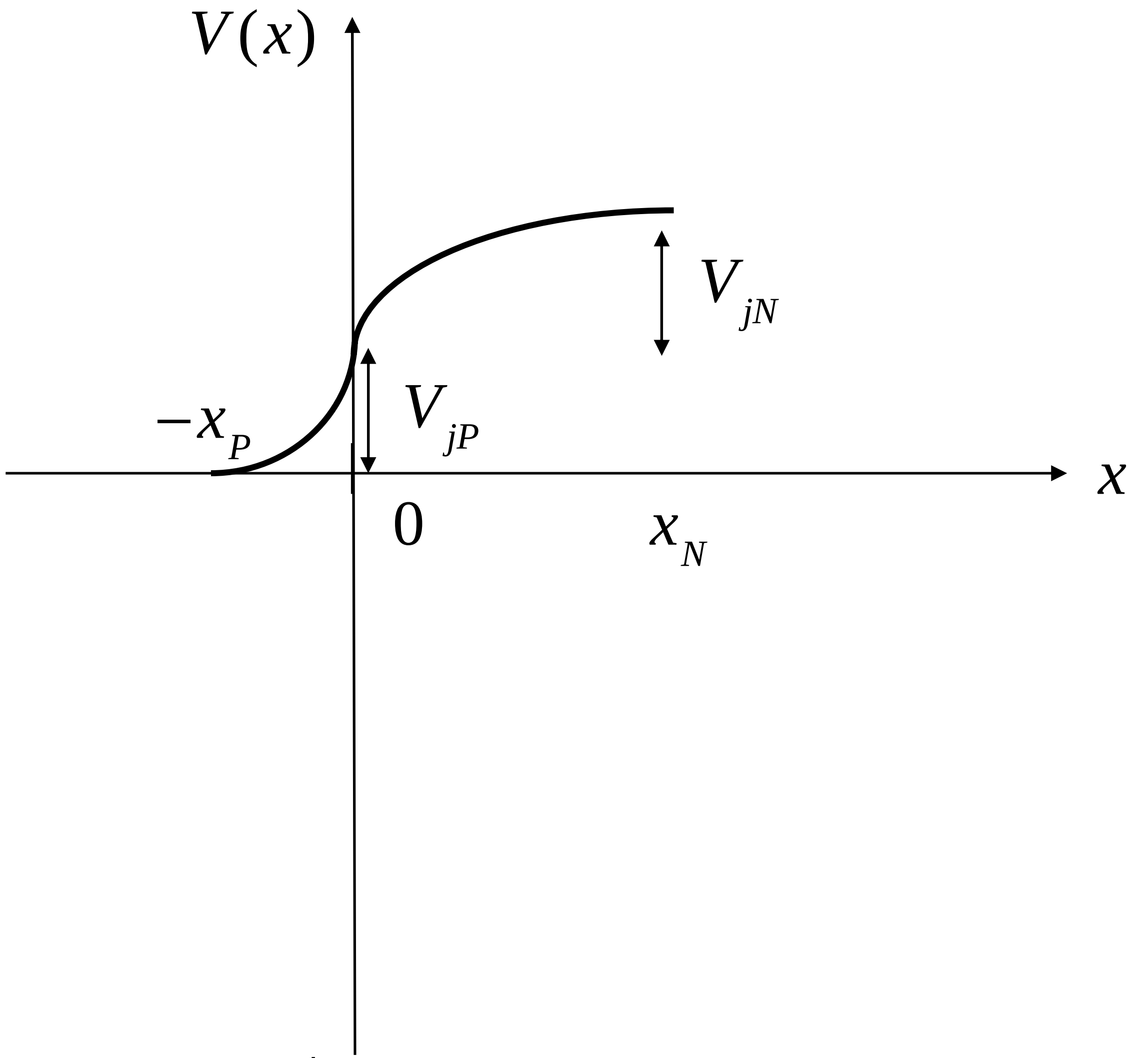


electric field

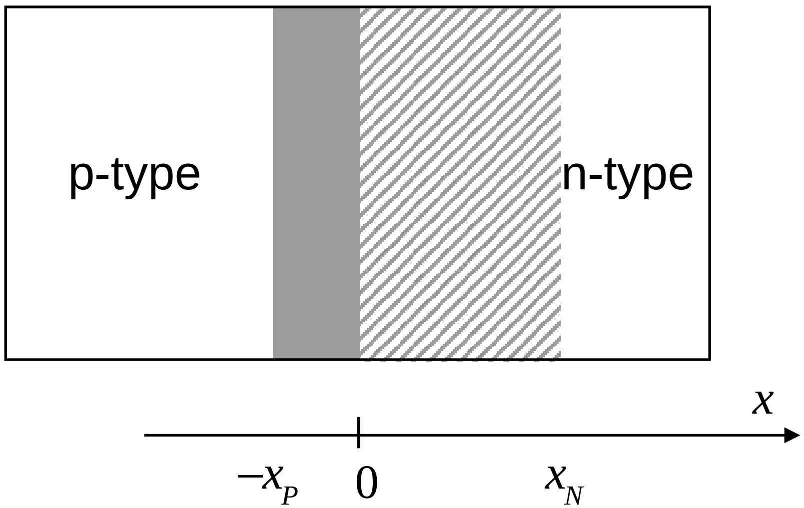


$$\varepsilon_P E\left(0^-\right) = \varepsilon_N E\left(0^+\right)$$

electrostatic potential



key results



$$E\left(0^-\right) = -qN_A x_P / \varepsilon_P$$

$$E\left(0^+\right) = -qN_N x_N / \varepsilon_N$$

$$V_{jP} = V_{BI}\, \varepsilon_N N_D / \left(\varepsilon_N N_D + \varepsilon_P N_A\right)$$

$$V_{jN} = V_{BI}\, \varepsilon_P N_A / \left(\varepsilon_N N_D + \varepsilon_P N_A\right)$$

$$V_{jP} / V_{jN} = \varepsilon_N N_D / \varepsilon_P N_A$$

$$x_P = \sqrt{2\varepsilon_P V_{jP} / qN_A}$$

$$x_N = \sqrt{2\varepsilon_N V_{jN} / qN_D}$$

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Poisson's equation for homostructures

$$\frac{d^2V}{dx^2} = -\frac{q}{\varepsilon}\left(p_o(x) - n_o(x) + N_D^+(x) - N_A^-(x)\right)$$

$$p_o(x) = n_i e^{(E_I - E_F)/k_B T} \qquad n_o(x) = n_i e^{(E_F - E_I)/k_B T}$$

$$E_I(x) = C - qV\left(x\right)$$

$$\frac{d^2V}{dx^2} = \frac{-q}{\varepsilon}\left(n_i e^{-qV/k_B T} - n_i e^{qV/k_B T} + N_D^+(x) - N_A^-(x)\right)$$

(Poisson-Boltzmann equation)

Poisson's equation for heterostructures

$$\frac{d^2V}{dx^2} = -\frac{q}{\varepsilon}\left(p_o(x) - n_o(x) + N_D^+(x) - N_A^-(x)\right)$$

$$-\varepsilon\frac{d^2V}{dx^2} \Longrightarrow \frac{d}{dx}\left(-\varepsilon\frac{dV}{dx}\right)$$

must relate *n*(*x*) and *p*(*x*) to *V*(*x*)

$$p_o(x) = N_V(x)e^{(E_V - E_F)/k_BT} \qquad n_o(x) = N_C(x)e^{(E_F - E_C)/k_BT}$$

$$E_C(x) = E_0 - \chi(x) - qV(x) \qquad E_V(x) = E_C(x) - E_G(x)$$

$$E_I(x) = E_0 - \chi(x) - E_G(x)/2 + (k_BT/2)\ln\left[N_V(x)/N_C(x)\right] - qV(x)$$

Poisson's equation for heterostructures

$$p_o(x) = n_{ir} e^{-q(V(x) - V_p(x))/k_B T}$$

$$qV_p(x) = \left(\chi(x) - \chi_{ref}\right) - \left(E_G(x) - E_{Gref}\right) + k_B T \ln\left[N_V(x) / N_{Vref}\right]$$

$$n_o(x) = n_{ir} e^{q(V(x) + V_n(x))/k_B T}$$

$$qV_n(x) = \left(\chi(x) - \chi_{ref}\right) + k_B T \ln\left[N_C(x) / N_{Cref}\right]$$

$$\frac{d}{dx}\left(-\varepsilon \frac{dV}{dx}\right) = q\left(n_{ir} e^{-q(V - V_p)/k_B T} - n_{ir} e^{q(V + V_n)/k_B T} - N_D^+ + N_A^-\right)$$

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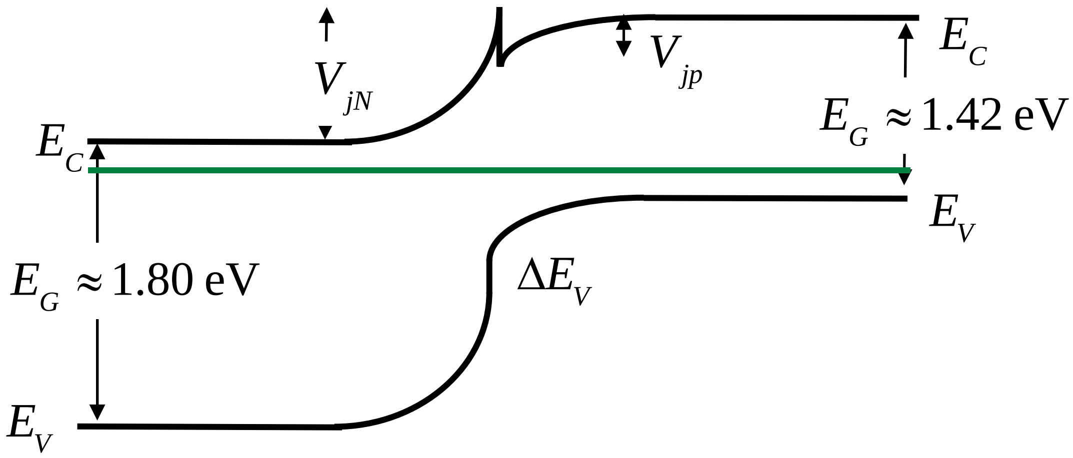
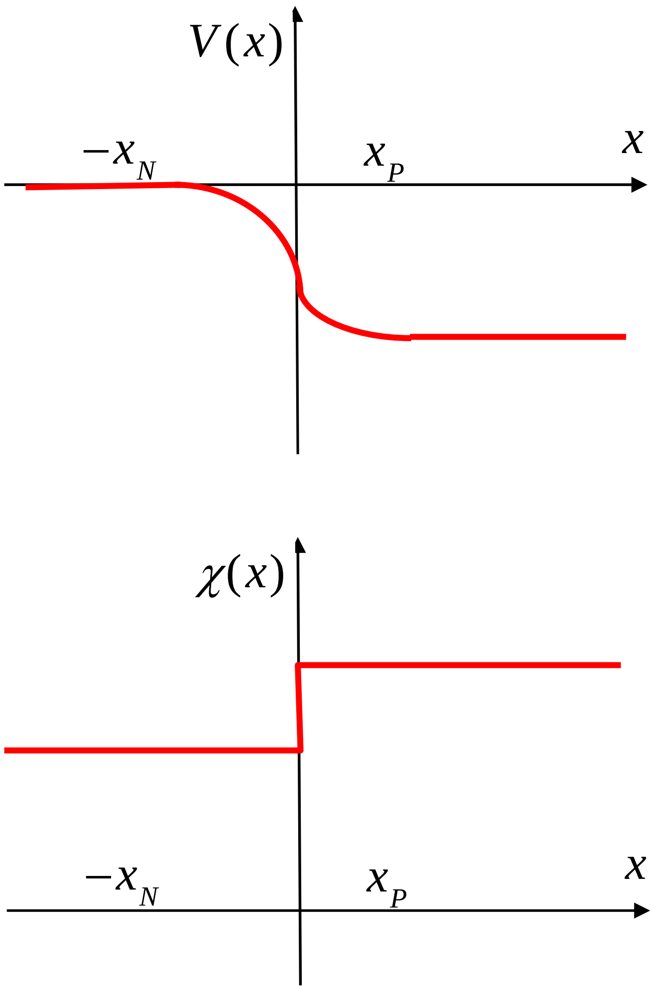
abrupt

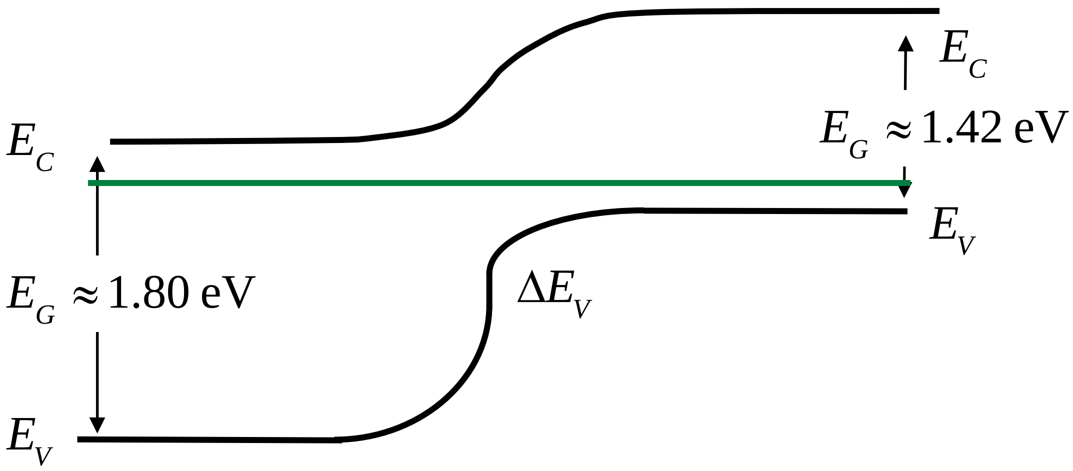




$$E_C(x) = E_0 - \chi(x) - qV(x)$$

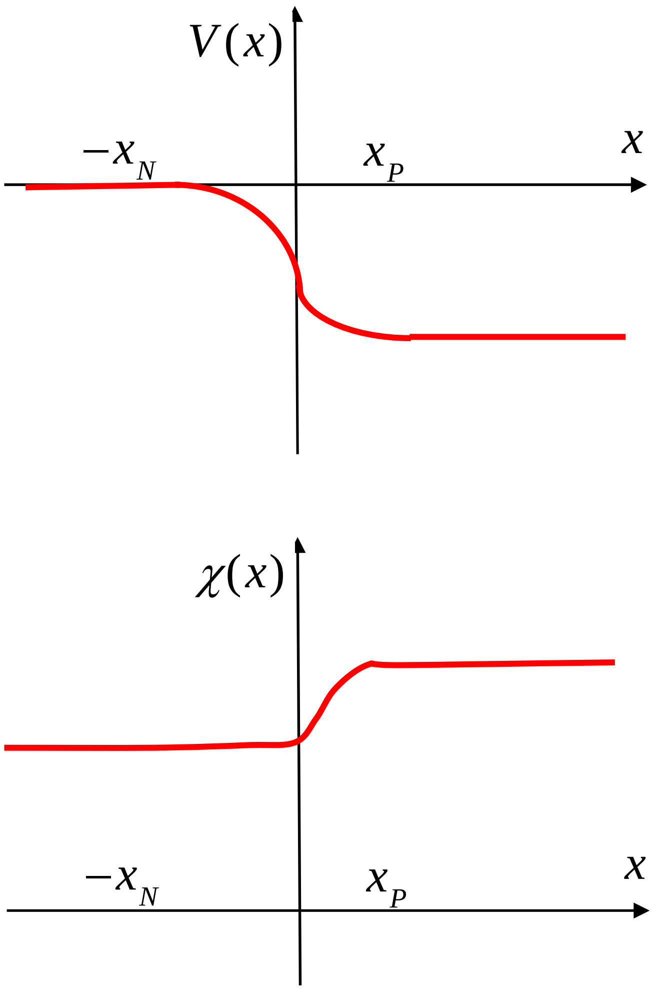
$$E_V(x) = E_C(x) - E_G(x)$$

graded

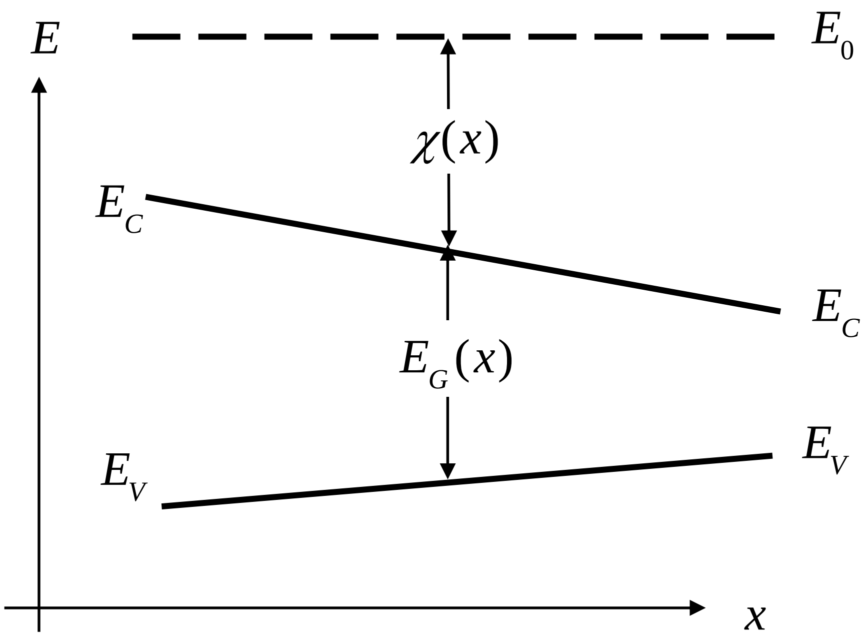


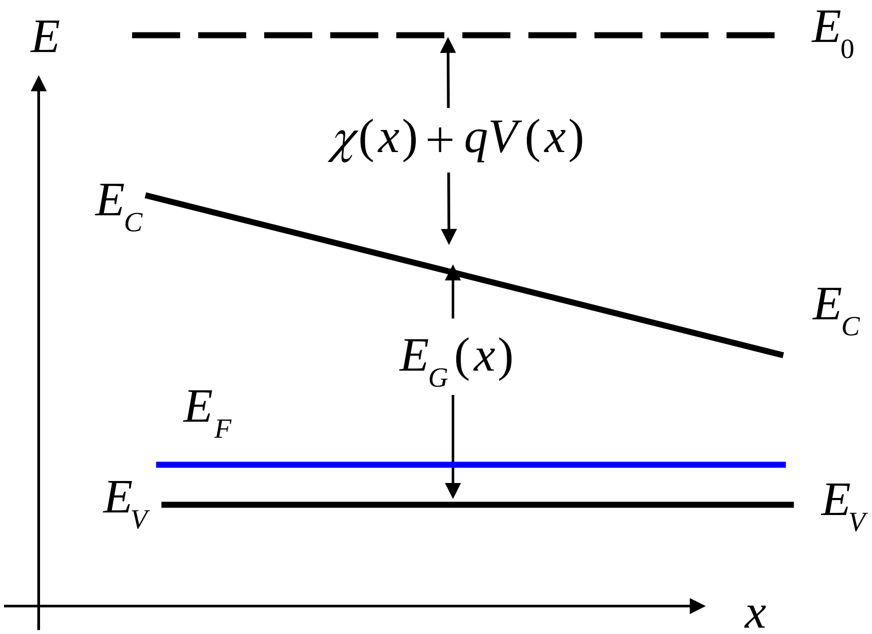
$$E_C(x) = E_0 - \chi(x) - qV(x)$$

$$E_V(x) = E_C(x) - E_G(x)$$



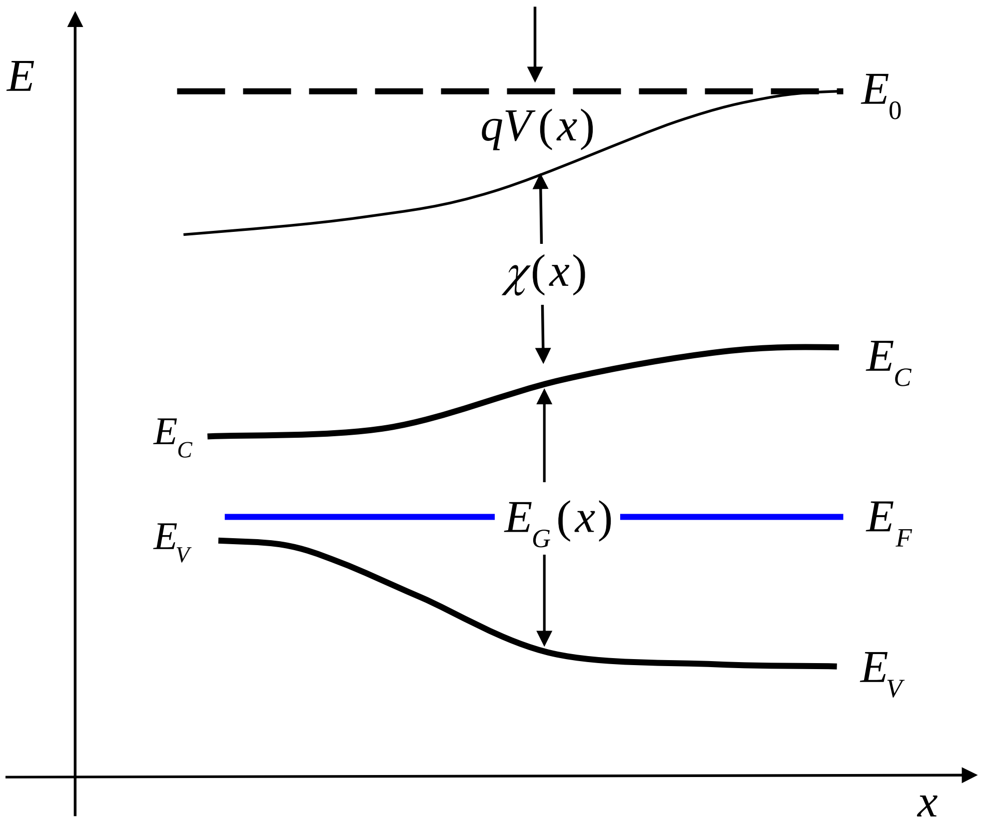
graded and quasi-neutral





uniformly p-doped

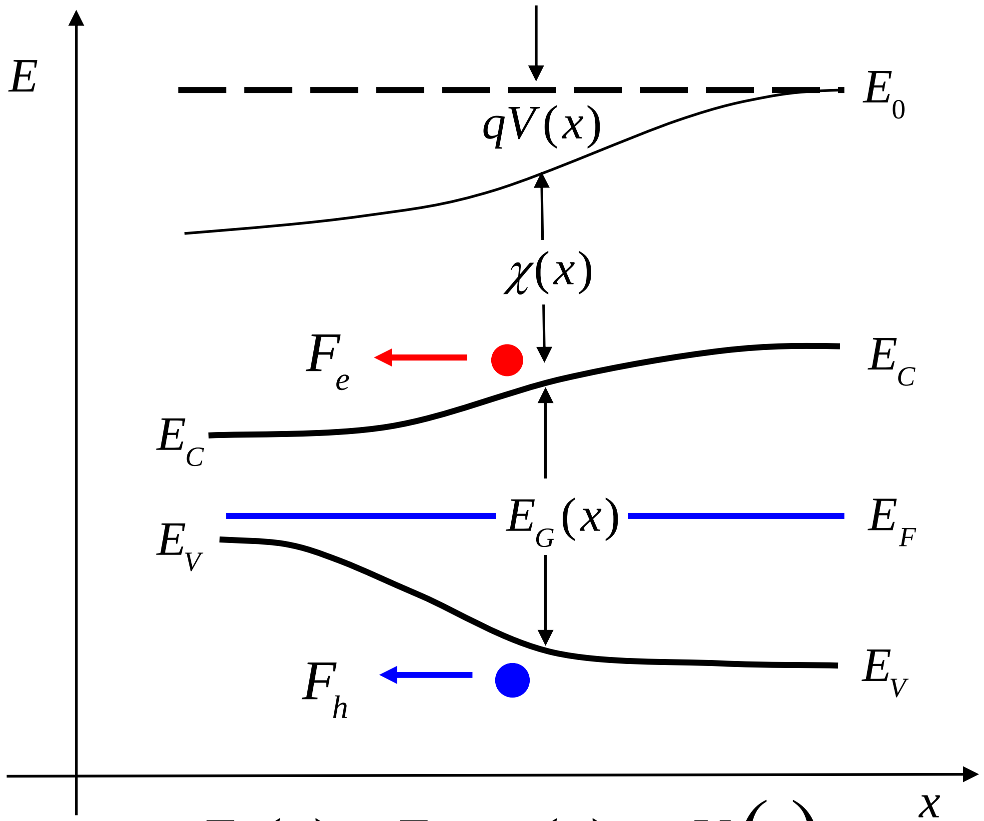
general, graded heterostructure



$$E_C(x) = E_0 - \chi(x) - qV(x)$$

$$E_V(x) = E_C(x) - E_G(x)$$

quasi-electric fields



$$E_C(x) = E_0 - \chi(x) - qV(x)$$

$$E_V(x) = E_C(x) - E_G(x)$$

$$F_e = -\frac{dE_C}{dx} = q\frac{dV}{dx} + \frac{d\chi}{dx}$$

$$F_e = -qE(x) - qE_{QN}(x)$$

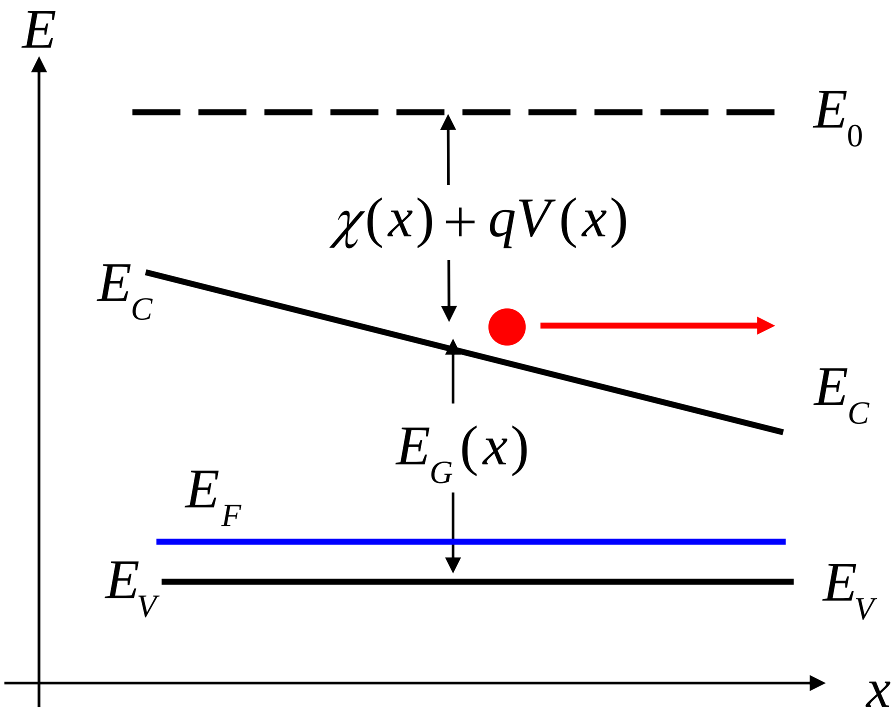
$$E_{QN} \equiv -\frac{1}{q}\frac{d\chi}{dx}$$

$$F_h = +\frac{dE_V}{dx} = -q\frac{dV}{dx} - \frac{d(\chi + E_G)}{dx}$$

$$F_h = +qE(x) + qE_{QP}(x)$$

$$E_{QP} \equiv -\frac{1}{q}\frac{d(\chi + E_G)}{dx}$$

graded and quasi-neutral



$$F_e = -qE(x) - qE_{QN}(x)$$

$$F_e = -\frac{dE_G(x)}{dx}$$

uniformly p-doped

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hole current

$$J_p = p\mu_p \frac{dF_p}{dx} \qquad p = N_V(x)\, e^{\left(E_V - F_p\right)/k_B T} \qquad F_p = E_V(x) - k_B T \ln\left(p/N_V\right)$$

$$\frac{dF_p}{dx} = \frac{dE_V(x)}{dx} - k_B T\left[\frac{1}{p}\frac{dp}{dx} - \frac{1}{N_V}\frac{dN_V}{dx}\right]$$

$$J_p = p\mu_p\left[\frac{dE_V(x)}{dx} + \frac{k_B T}{N_V}\frac{dN_V}{dx}\right] - k_B T \mu_p \frac{dp}{dx}$$

$$\frac{dE_V(x)}{dx} = \frac{d}{dx}\left[E_0 - \chi(x) - E_G(x) - qV(x)\right] = q\left(\mathcal{E}(x) + E_{QP}\right)$$

hole and electron currents

$$J_p = pq\mu_p\left[E + E_{QP} + \frac{k_B T}{q}\frac{1}{N_V}\frac{dN_V}{dx}\right] - qD_p\frac{dp}{dx}$$

'DOS effect'

$$J_n = nq\mu_n\left[E + E_{QN} - \frac{k_B T}{q}\frac{1}{N_C}\frac{dN_C}{dx}\right] + qD_n\frac{dn}{dx}$$

quasi-electric fields

$$E_{QP} \equiv -\frac{1}{q}\frac{d\left(\chi + E_G\right)}{dx} \qquad E_{QN} \equiv -\frac{1}{q}\frac{d\chi}{dx}$$

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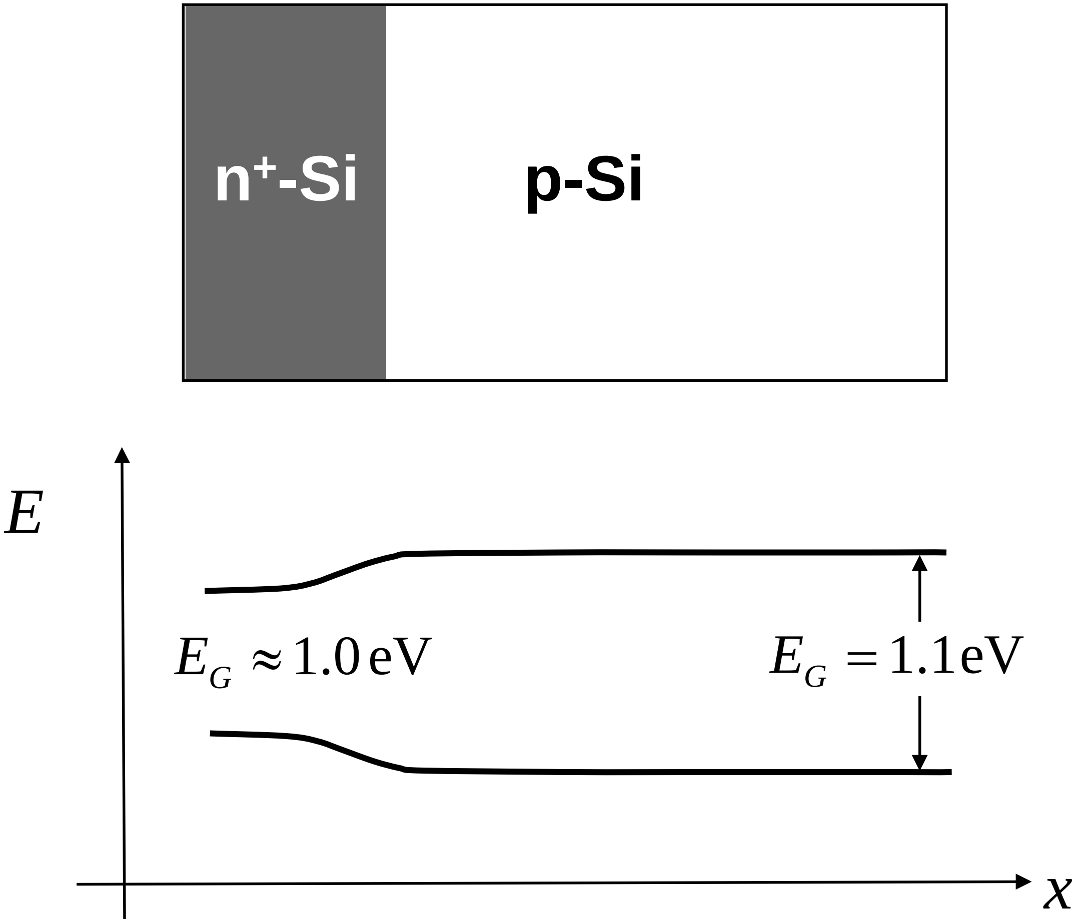
bandgap shrinkage



$$n_i^2(x) = n_i^2 e^{\Delta_G / k_B T}$$

DD equations with bandgap shrinkage

$$n_i^2(x) = n_i^2 e^{\Delta_G / k_B T}$$

$$J_p = pq\mu_p \left[E + \frac{d\left[\left(1-\gamma\right)\Delta_G\right]}{dx} \right] - qD_p \frac{dp}{dx}$$

$$J_n = nq\mu_n \left[E - \frac{d\left(\gamma \Delta_G\right)}{dx} \right] + qD_n \frac{dn}{dx}$$

(γ = 0.5 is typically assumed)

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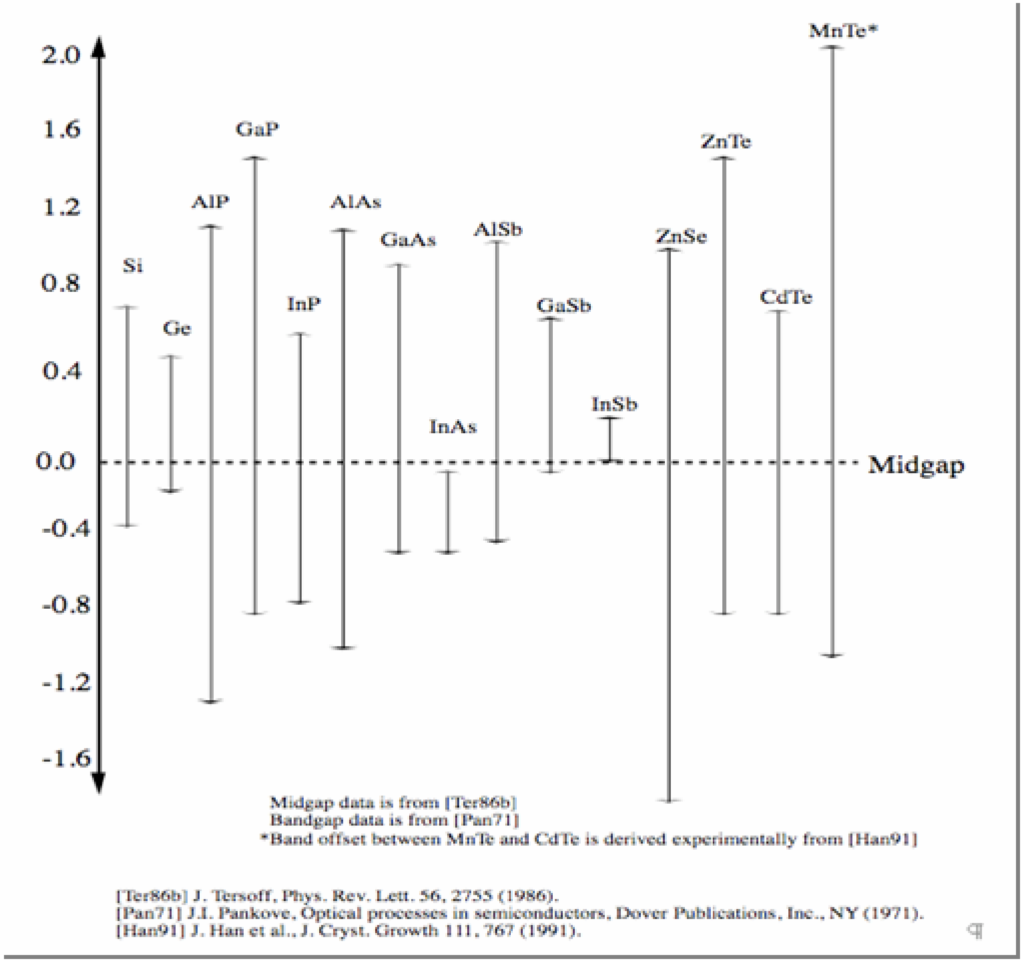
measured offsets



(courtesy Jung Han, Purdue Univ., 1995)

determining offsets

1) electron affinity rule:

- $\Delta E_C = \chi_1 - \chi_2$
- χ ~ 4 eV (surface charges, orientations, etc.)
- semi-semi dipole vs. semi-vacuum dipole

2) **common anion rule:**

- AlGaAs / GaAs
- valence band offset should be smaller than conduction band

3) **Tersoff theory:**

- gap states produced at interface
- lead to an interface dipole
- bands adjust to minimize dipole
- explains Schottky barrier heights too.

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