6.730 Physics for Solid State Applications

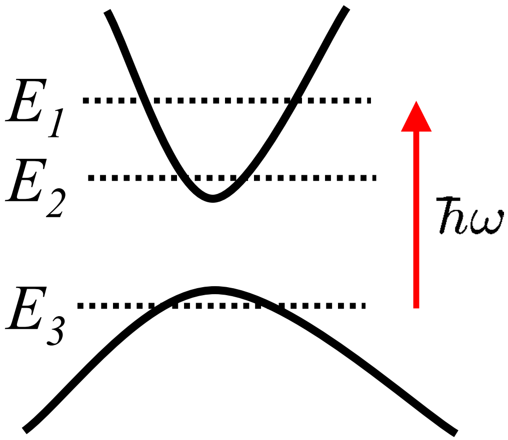
Lecture 26: Inhomogeneous Solids

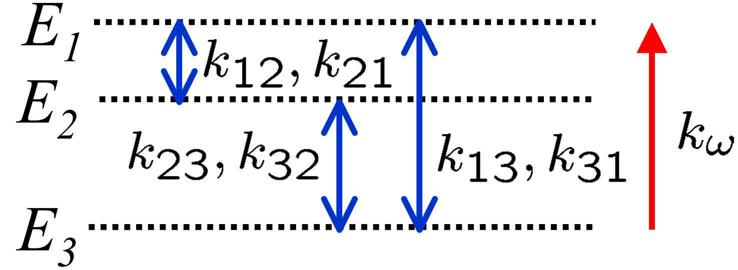
Outline

- Last Time: Quasi-Fermi Levels
- Inhomogenous Solids in Equilibrium
- Quasi-equilibrium Transport
- Heterostructures

Near Equilibrium Electron Distributions

Optical Excitation





k_{12}, k_{21}	Intraband scattering:	electron-electron electron-acoustic phonon
k_{23}, k_{32} k_{13}, k_{31}	Interband scattering:	electron-hole electron-phonon with defects

What are f_1, f_2, & f_3 under illumination (non-equilibrium) ?

Steady-State Solutions
Non-equilibrium

$$\frac{dn_3}{dt} = \frac{dn_1}{dt} = \frac{dn_2}{dt} = 0$$

$$\frac{f_1(1-f_2) - A_{12} f_2 (1-f_1)}{f_2(1-f_3) + A_{23} f_3 (1-f_2)} = \frac{k_{23}}{k_{12}} \frac{N_3}{N_1}$$

For example when intraband scattering is much faster than interband scattering…

$$N_1 \sim N_3 \qquad k_{12} \gg k_{31}, k_{23}$$

$$f_1(1-f_2) - A_{12} f_2 (1-f_1) \approx 0$$

$$\frac{f_1}{(1-f_1)} \approx A_{12} \frac{f_2}{(1-f_2)}$$

Steady-State Solutions
Non-equilibrium

Equilibrium Fermi-Dirac distribution:

$$f^o(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)}$$

Non-equilibrium Quasi-Fermi-Dirac distribution:

$$f_i(E_i) = \frac{1}{1 + \exp\left(\frac{E_i - E_{F_i}}{k_B T}\right)}$$

$$\frac{f_1}{(1 - f_1)} \approx A_{12} \frac{f_2}{(1 - f_2)}$$

$$e^{-(E_1 - E_{F_1})/k_B T} \approx e^{-(E_1 - E_2)/k_B T} \, e^{-(E_2 - E_{F_2})/k_B T}$$

$$E_{F_1} \approx E_{F_2}$$

Intraband states have same chemical potential

⇨ in 'equilibrium' with each other because of fast intraband scattering

Steady-State Solutions

Non-equilibrium

$$N_1 \frac{df_1}{dt} \to 0 = -k_{12}\, N_1\, N_2\, [f_1(1-f_2) + A_{12}\, f_2\, (1-f_1)]$$

$$-k_{13}\, N_1\, N_3\, [f_1(1-f_3) + A_{13}\, f_3\, (1-f_1)] + k_\omega\, N_3\, N_1 f_3 (1-f_1)$$

$$E_{F_3} = E_{F_1} - k_B T \ln \left[\frac{k_\omega e^{(E_1 - E_3)/k_B T} + A}{A} \right]$$

$$A = k_{13} + \frac{N_2}{N_1} k_{21} e^{(E_1 - E_2)/k_B T}$$

Interband states have different chemical potentials

unless $k_\omega \to 0$ $E_{F_3} = E_{F_1}$

Counting in Non-equilibrium Semiconductors

Equilibrium

$$N_o = N_c \exp\left(\frac{-(E_c - E_{F_o})}{k_B T}\right)$$

$$P_o = N_v \exp\left(\frac{-(E_{F_o} - E_v)}{k_B T}\right)$$

$$N_o P_o = N_c N_v \exp\left(\frac{-E_g}{k_B T}\right) = N_i^2$$

Quasi-equilibrium

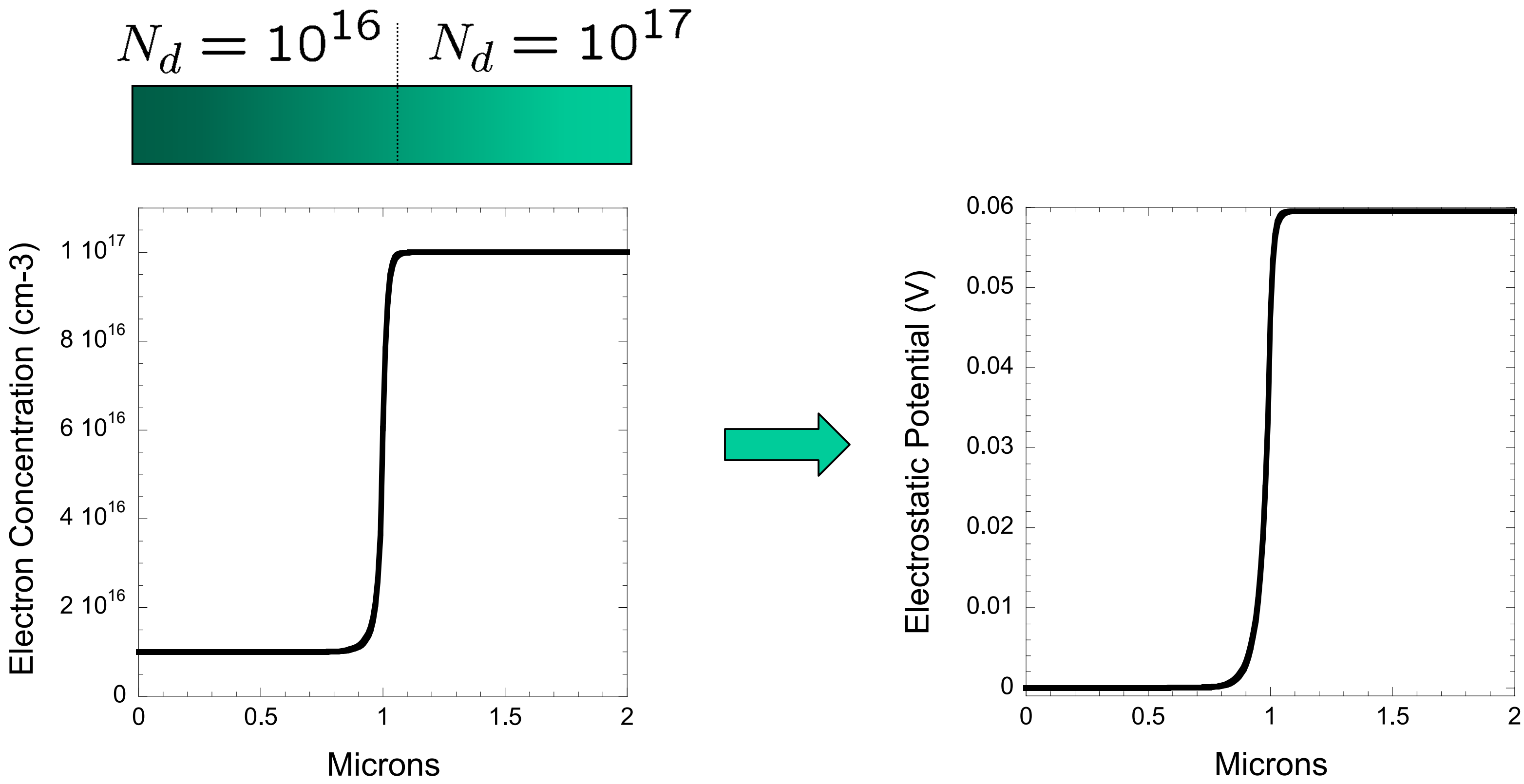
$$N \approx N_c \exp\left(\frac{-(E_c - E_{F_c})}{k_B T}\right)$$

$$P \approx N_v \exp\left(\frac{-(E_{F_v} - E_v)}{k_B T}\right)$$

$$N P = N_i^2 \exp\left(\frac{-(E_{F_c} - E_{F_v})}{k_B T}\right)$$

Inhomogeneous Semiconductors in Equilibrium

Consider a solid with a spatially varying impurity concentration…



In equilibrium, the carrier concentration is balanced by an internal electrostatic potential…

Inhomogeneous Semiconductors in Equilibrium

If electrostatic potential varies slowly compared to wavepacket…

$$\left(-\frac{\hbar^2\nabla^2}{2m^*} + E_{co} - q\phi(r)\right) G(r) = E G(r)$$

Dividing solid into slices where ϕ_i is uniform…

$$-\frac{\hbar^2\nabla^2}{2m^*} G_i(r) = \left(E_i - E_{co} + q\phi_i\right) G_i(r)$$

…the envelope function has solutions of the form…

$$G_i(r) = \left(A_i e^{ik_x x} + B_i e^{-ik_x x}\right) e^{+ik_y y} e^{+ik_z z}$$

…therefore the eigenenergies are…

$$E_i = E_{co} - q\phi_i + \frac{\hbar^2 k^2}{2m^*} \quad \Longrightarrow \quad E(r) = E_{co} - q\phi(r) + \frac{\hbar^2 k^2}{2m^*}$$

Inhomogeneous Semiconductors in Equilibrium

Given the modified energy levels, the 3-D DOS becomes….

$$g(E,r) = \frac{1}{2\pi^2\hbar^3}(2m^*)^{3/2}\left[E - E_{co} + q\phi(r)\right]^{1/2}$$

…in equilibrium the carrier concentration is…

$$N_o(r) = \int_{E_{co}-q\phi(r)}^{\infty} g(E,r)\frac{1}{1+e^{(E-E_{F_o})/k_BT}}dE$$

$$N_o(r) = \frac{2}{\sqrt{\pi}}N_c\,F_{1/2}\left(\frac{E_{F_o} - E_{co} + q\phi(r)}{k_BT}\right)$$

Boltzmann approx. $\approx N_c \exp\left(\frac{-(E_{co} - q\phi(r) - E_{F_o})}{k_BT}\right)$

Inhomogeneous Semiconductors in Equilibrium

$$N_o(r) = \frac{2}{\sqrt{\pi}} N_c \, F_{1/2}\left(\frac{E_{F_o} - E_{co} + q\phi(r)}{k_B T}\right)$$

$$\approx N_c \exp\left(\frac{-(E_{co} - q\phi(r) - E_{F_o})}{k_B T}\right)$$

$$E_c(r) \equiv E_{co} - q\phi(r)$$

$$N_o(r) = \frac{2}{\sqrt{\pi}} N_c \, F_{1/2}\left(\frac{E_{F_o} - E_c(r)}{k_B T}\right)$$

$$\approx N_c \exp\left(\frac{-(E_c(r) - E_{F_o})}{k_B T}\right)$$

The slowly varying electrostatic potential can be incorporated in $E_c(r)$

Quasi-equilibrium Transport

$$N(r) \approx N_c \exp\left(\frac{-(E_c(r) - E_{F_c})}{k_B T}\right) \Rightarrow E_{F_c} = E_c(r) + k_B T \ln \frac{N(r)}{N_c}$$

$$E_c(x) = E_{co} - q\phi(x)$$

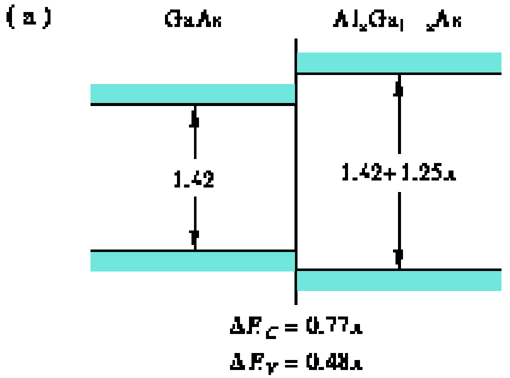
$$\frac{dE_c(x)}{dx} = -q\frac{d\phi(x)}{dx} = qE_x$$

$$\begin{aligned}
J_{n_x} &\approx \mu_n N \frac{dE_{F_c}}{dx} \\
&= \mu_n N \frac{dE_c}{dx} + \mu_n k_B T \frac{N_c}{N} \frac{1}{N_c} \frac{dN}{dx} \\
&= \mu_n N \frac{dE_c}{dx} + \mu_n k_B T \frac{dN}{dx} \\
&= \mu_n N qE_x + \mu_n k_B T \frac{dN}{dx}
\end{aligned}$$

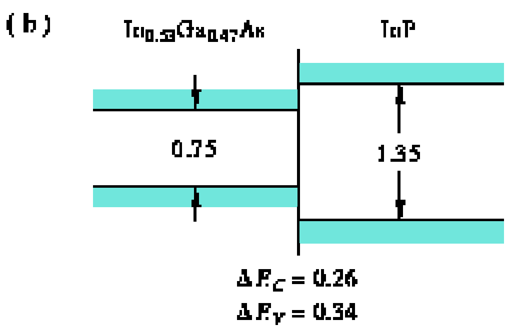
$$J_{n_x} \equiv q\mu_n N E_x + qD_n \frac{dN}{dx}$$

Species of Heterjunctions

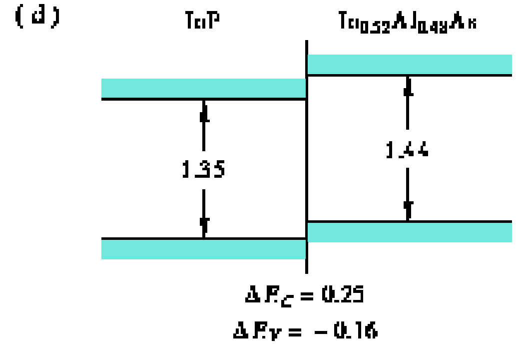
Type I



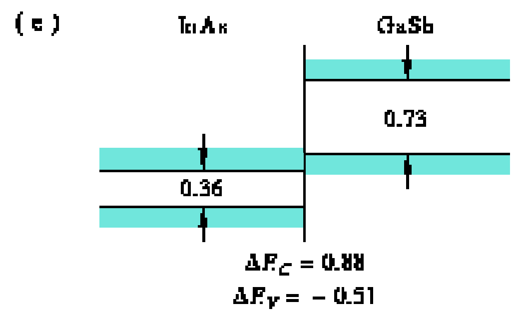
Type I



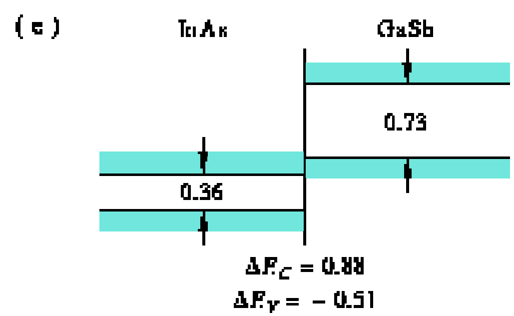
Type II



Type III



Type III

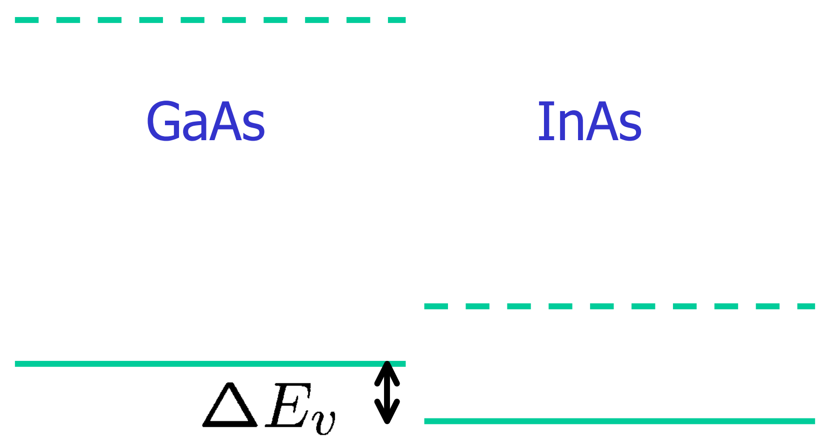


http://www.utdallas.edu/~frensley/technical/hetphys

Tight-binding Calculation of Band Alignments

LCAO internally references bandstructures to each other…

$$E_v(k=0) = \frac{E_p^1 + E_p^2}{2} - \sqrt{\left(\frac{E_p^1 - E_p^2}{2}\right)^2 + \left(\frac{1.28\hbar^2}{md^2}\right)^2}$$



Unfortunately, this doesn’t take into account the details of the charges and bonding at the interface…

…need a self-consistent LCAO theory…still a research topic !

Tight-binding Calculation of Band Alignments

$$E_v(k=0) = \frac{E_p^1 + E_p^2}{2} - \sqrt{\left(\frac{E_p^1 - E_p^2}{2}\right)^2 + \left(\frac{1.28\hbar^2}{md^2}\right)^2}$$

Example GaAs/InAs

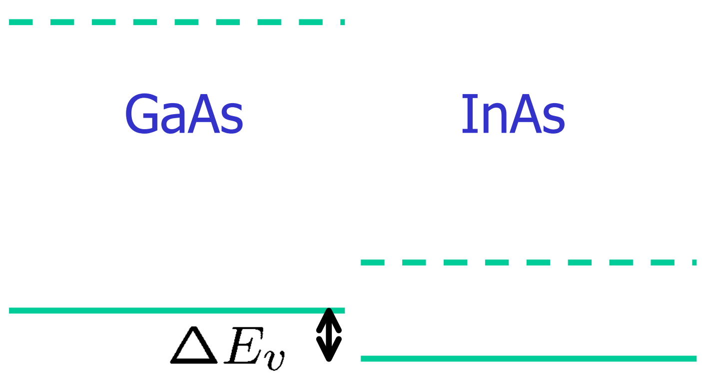
Ga: $E_p = -4.9\,\text{eV}$ As: $E_p = -7.91\,\text{eV}$ In: $E_p = -4.69\,\text{eV}$

GaAs: $d = 2.45\,\text{A}$

$E_v = -8.61\,\text{eV}$

InAs: $d = 2.61\,\text{A}$

$E_v = -8.45\,\text{eV}$

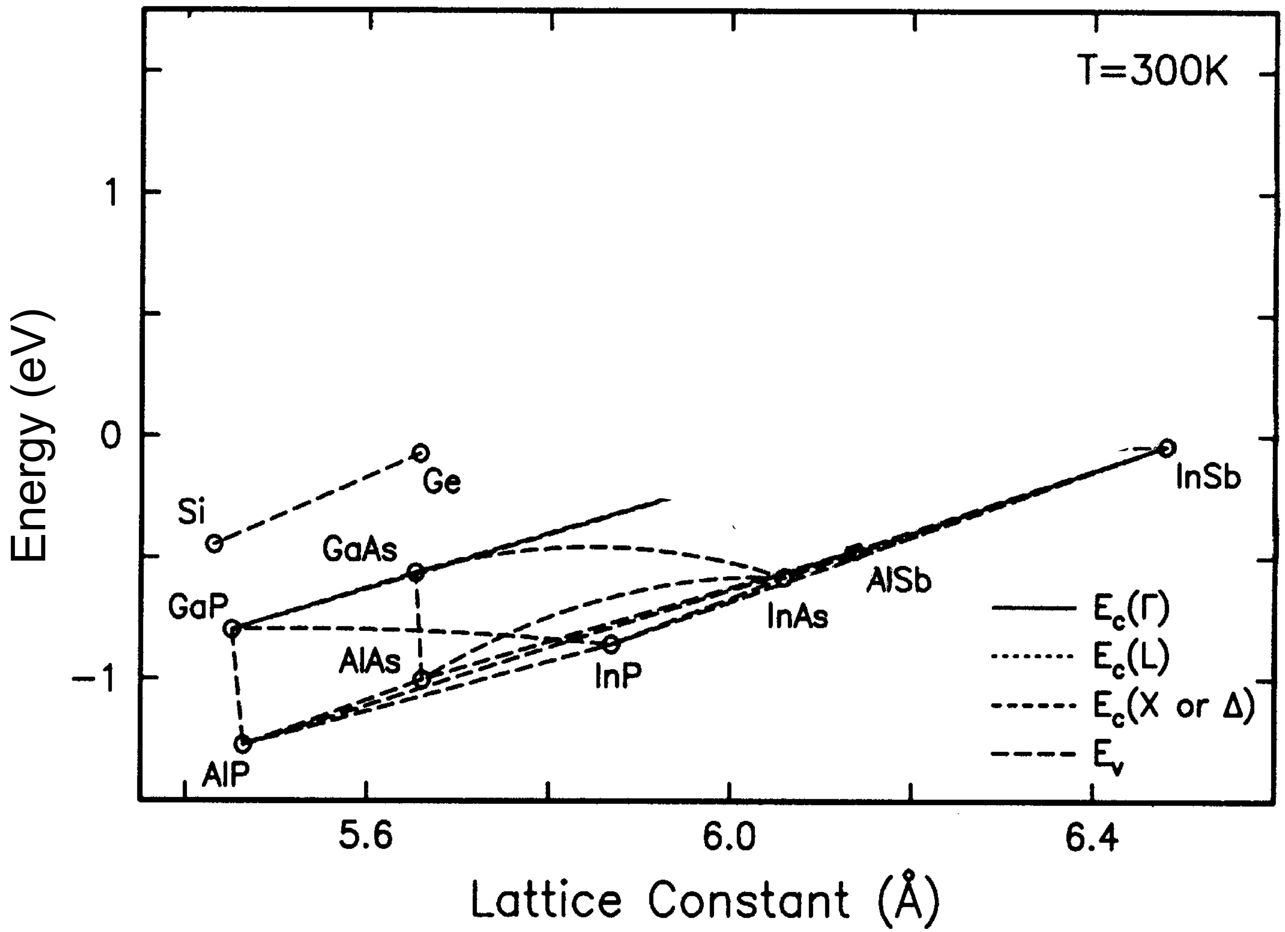


GaAs/InAs: $\Delta E_v = 0.16\,\text{eV}$ (LCAO)

$\Delta E_v = 0.17\,\text{eV}$ (experiment)

Experimentally Determined Band Alignment

Valence Band Alignment



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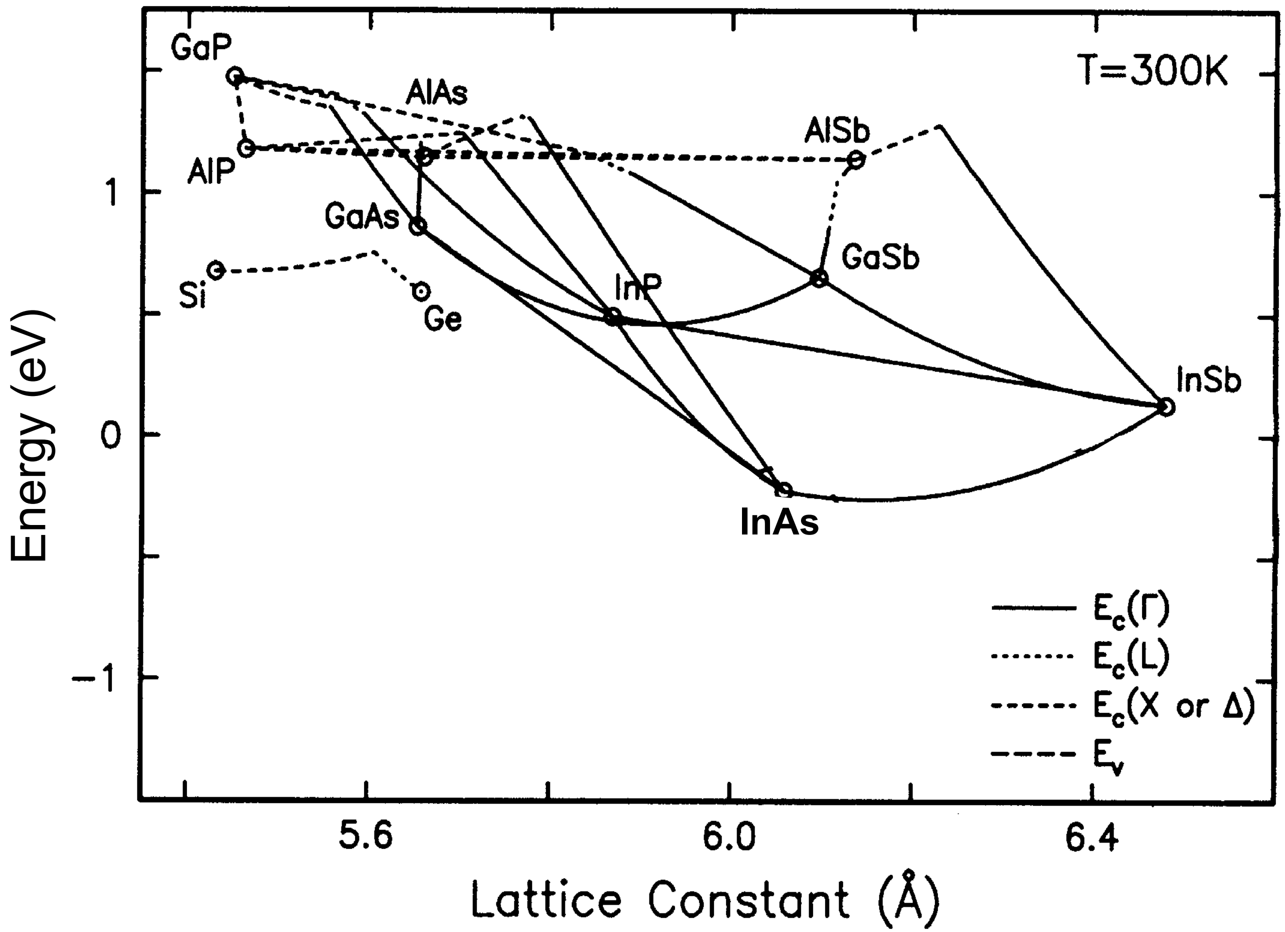
Experimentally Determined Band Alignment

Conduction Band Alignment



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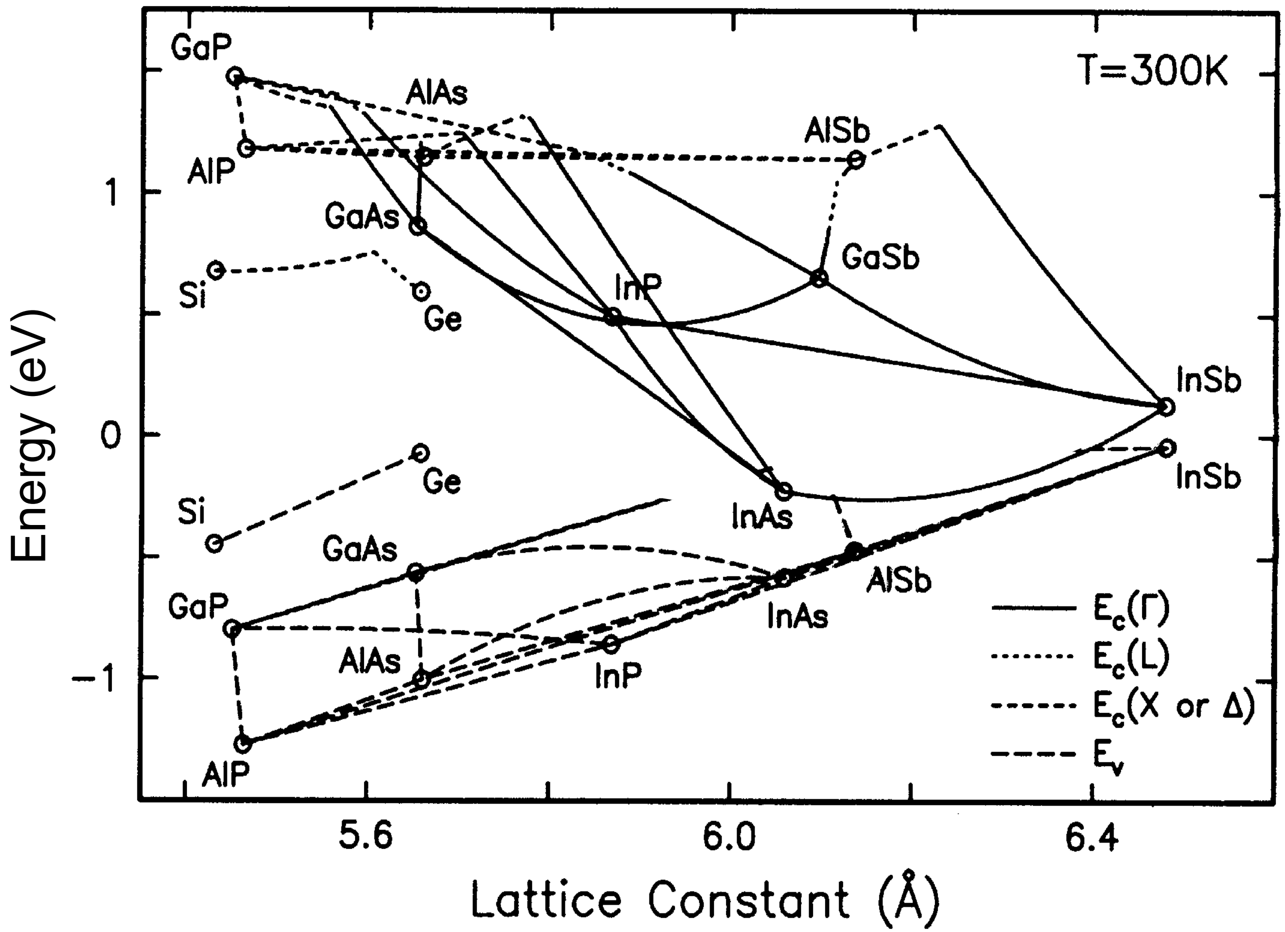
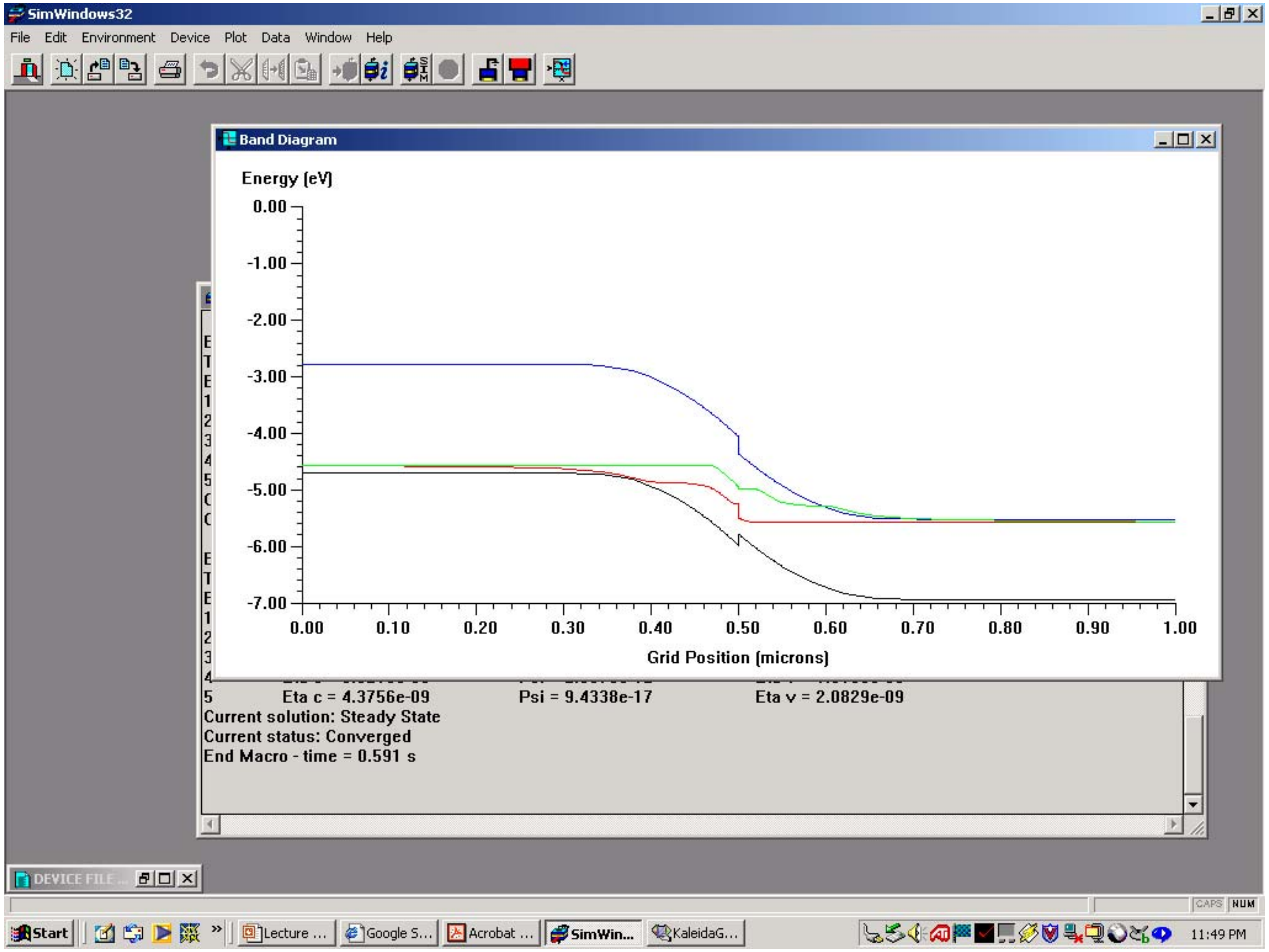
Experimentally Determined Band Alignment



SimWindows Software

Self-consistent solution of *modified* drift-diffusion & Poisson's Equation…



http://www-ocs.colorado.edu/SimWindows/simwin.html