

**Problem solutions are to be turned in at the beginning of class on the due date. Solutions to all problems will be provided after problem sets are collected in class. SHOW ALL WORK.**

1. Consider GaAs at 300K, which has the cubic zincblende crystal structure and a cubic lattice constant  $a=5.65\text{\AA}$ . In all cases you may assume flat-band conditions within each material.
  - (a) GaAs forms a Type I heterojunction interface with  $\text{Al}_x\text{Ga}_{1-x}\text{As}$ , which has a larger energy band gap. Suppose that for a given composition of the  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  alloy,  $\Delta E_c = 0.3\text{eV}$  and  $\Delta E_v = 0.2\text{eV}$ . Draw the resulting energy band edge diagram for the GaAs/ $\text{Al}_x\text{Ga}_{1-x}\text{As}$  heterojunction.
  - (b) Suppose a dipole consisting of two sheets of charge equal in magnitude but opposite in sign is present right at the heterojunction interface. The sheet charges are separated by a distance of one cubic lattice constant. The charge density magnitude on each sheet is  $\sigma = 1 \times 10^{13} q / \text{cm}^2$ , where  $q$  is the magnitude of the electron charge, and the positive charge is on the GaAs side of the interface. Compute the band offsets (give numerical values) in the presence of this interface dipole and draw the resulting energy band edge diagram, assuming the band offset values in part (a) are in the absence of any interface dipole. You may assume the dielectric constant throughout the heterojunction to be that of GaAs,  $\epsilon = 12.9\epsilon_0$ .
  - (c) Suppose the heterojunction interface lies in the (100) plane. For the charge density given in part (b), compute the charge per atom (give either a numerical value or a fraction of  $q$ ) in the (100) plane corresponding to the positive sheet charge density in part (b).
  
2. Consider a heterojunction between two semiconductor materials, A and B, whose electron affinities are equal. Their energy band gaps are  $E_g^A = 1.00\text{eV}$  and  $E_g^B = 2.00\text{eV}$ . The cubic lattice constant may be assumed to be  $a = 6.00\text{\AA}$  for each material, and the dielectric constant to be  $10\epsilon_0$  throughout the heterojunction. In all cases you may assume flat-band conditions within each material.
  - (a) Draw the energy band edge diagram and compute  $\Delta E_c$  and  $\Delta E_v$  for this heterojunction, assuming that the electron affinity rule is valid.
  - (b) Now suppose that both materials have a “midgap” energy at the exact midpoint of their energy band gaps, and that in each material a deviation of the Fermi level from the “midgap” energy at a heterojunction interface produces a charge density at the interface of  $-\sigma(E_F - E_{\text{midgap}})$  with  $\sigma = 1 \times 10^{14} q / \text{cm}^2 \cdot \text{eV}$ . Assume that these charges in each material are separated from each other by one cubic lattice constant at the heterojunction interface. By requiring overall charge neutrality in the heterojunction and consistency of the heterojunction dipole with the band offset, compute the numerical values of the conduction-band and valence-band offsets and draw the resulting energy band edge diagram. You should assume that in the absence of any interface dipole, the electron affinity rule is valid. While this model is overly simplistic, it captures some of the effects of so-called midgap alignment energies.