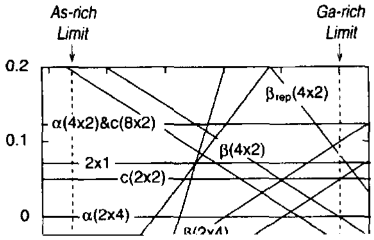
is such that (i) the surface band gap levels are

atomic sites charge-compensate each other. In the simplest cases, these atomic sites form charge-com

where each term is a difference with respect to σ_0.

chemical potential, μ_{Ga} and μ_{As}, and not a function of the electron chemical potential, μ, due to surface



and identical motifs frequencies $\{\omega_M\}$ (i.e., chemically identical). As a consequence, in constructing the AI + AII grooves and the double A steps from the $\beta 2(2\times 4)$ surface, we do not need to transfer any atom between the surfaces and atomic reservoirs. In other words, the formation energies of the AI + AII grooves and the double A steps from the parent dimer are indistinguishable, thus each contributes