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bond orbitals of Ga ~3:' and As ~:3~ and the Ga-Ga and As-As "wrong bonds" are shaded, b~;. and bA~ denote "Ga-Ga" and "'As-As"

endothermic. There are two commonly observed steps: "electronic additions" (i.e. surface adatoms or vacangiar) that land to algertranic componention and thus to

principles the total energies of various flat surface structures [12-14], and to some degree the relative to some degree the relative to some degree the relative of energies of different step structures [15], these types of

In fact, in a relatively large collection of  $(0,1)$  surface collection of  $(0,0)$ 

named here "structural motifs". Using the superscript "structural motifs". Using the superscript "structural m (ii) to denote the coordination number, the structural interaction number, the structural interaction  $\mathcal{L}_\text{c}$ motifs include (Fig. 1) tetrahedrally bonded Ga/4) and  $A$  , pyramidal  $A$  is planet for  $\mathcal{A}$  is planet for  $\mathcal{A}$  is planet for  $\mathcal{A}$  $\mathcal{L}_{\mathcal{L}}$  , with bond angles of 109.5  $\mathcal{L}_{\mathcal{L}}$  , 120  $\mathcal{L}_{\mathcal{L}}$  , 120  $\mathcal{L}_{\mathcal{L}}$ respectively. A close examination of the actual atomic

dicular to the As dimers (B steps). The As dimers (B steps). The As dimers (B steps).

stable and semiconducting flat surfaces. While

Previous studies of  $GaAs(001)$  surfaces [17] roughlad that t<u>he eater rule tends to be cheved by these</u> near the conduction band minimum (CBM) so as to a

completely full or completely empty so that the systems remain semiconducting. This octet shell (fully occupied or fully empty levels) is necessary, but not sufficient, to

Ga/3~ with the As/3! we can achieve charge neutrality

the energy gap). Total energy calculations indeed tend to produce surface surface surface structures that reflect surface surface surface surface surface surface sur competitive functions  $\mathcal{I}_1$  and  $\mathcal{I}_2$  are centred demonstrated by  $\mathcal{I}_2$ strated  $\mathcal{I}_1$  that such a charge compensation-electron-electron-electron-electron-electron-electron-electron-electron-electron-electron-electron-electron-electron-electron-electron-electron-electron-electron-electroncounting model can be used in a quantitative fashion to explain the order of surface energies in flat GaAs(001)

motifs, leading to a set of point charges on various on various charges on various charges on various charges

stable and semiconducting flat surfaces. While step-step interaction has noticeable effects on step formation energies, the formation of steps is generally endothermic. There are two commonly observed steps: those with edges por led the direction of currence As motifs, leading to a set of point charges on various surface atoms. For example, Ga has 3 valence electrons, so fourfold coordinated  $Ga^{(4)}$  contributes 3/4 electrons to each of its four bonds. This leads to local charge noutrality  $P_{\text{RIP}} C_n(3)$  is  $n-2/4$  also<br>treat donor

As mentioned in Section 3.4, Heller et al.  $[5]$  have measured step energy by way of measuring the kink distribution on  $GaAs(001)$ -2×4. Depending on  $\frac{1}{2}$  energy ratio to be  $\frac{1}{2}$ ,  $\frac{1$ competature, they columned an  $\lambda$  step formation energy

temperature, they obtained an A step formation energy in the range from 14 to 20 meV/(1  $\alpha$  ) (these energies energies energies energies energies energies energies include also the corner energies in Reg. [5]). Following

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include also the corner energies in Ref. [5]). Following Heller et al., one may derive from the calculated kink energy in Section 3.4 the A step formation energy. This gives  $28-31$  meV/ $(1 \times)$ . Heller et al. also determined the B:A energy ratio to be  $5.6-6$ . Ide et al. [7], on the contrary, estimated the ratio from measured aniso-

## **References**

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