

-001! surface having the same projected -001! area. Because the concentration of H is different in each phase, and because steps can introduce a local change of the H density with respect to the flat surface, both the surface and step formation energies are functions of the H chemical potential m_H . In Fig. 1, the highest value of m_H -taken here as zero! is that at which H extracts without energy cost Si atoms from the surface, forming the SiH_4 molecules.²¹

III. FLAT SURFACE

Figure 1 shows schematically calculated surface formation energies of clean Si-001! @Fig. 1-a!# and hydrogenated Si-001! @Fig. 1-b!#

reduces the steric energy. This effect is not present at the $S_{\perp}^* \uparrow S_{\parallel}^*$ structure (see Fig. 2-a!). Accordingly, the formation energy of the *isolated* S_{\perp}^* might be one-tenth of an eV higher than the one estimated here from $S_{\perp}^* \uparrow S_{\perp}^*$.

Figure 2-c! shows the D_{\perp}^* step with a dihydride configuration similar to S_{\perp}^* (see row *a* in Figs. 2-c! and 2-a!). In contrast to S_{\perp}^* , we find that $\Delta E(D_{\perp}^*) < 0$. Since the upper terraces of D_{\perp}^* and S_{\perp}^* have similar structures, one might wonder why the energy costs of the steps are so different. The reasons are the following. -i! The estimated $\Delta E_{\text{bare}}(D_{\perp}^*)$ is close to twice $\Delta E_{\text{bare}}(S_{\parallel}^*)$. -ii! The structure used to calculate D_{\perp}^* does not involve the partition of the dimer rotation angles seen in $S_{\perp}^* \uparrow S_{\perp}^*$. -iii! On the D_{\perp}^*

formation energy of $S_{\perp}^* \uparrow S_{\perp}^*$ to estimate $\Delta E(S_{\perp}^*) \approx 0.27$ eV/a. The reasons for a negative formation energy of S_{\perp}^* are twofold: -i! Steric energy reductions at the step edge: One may write the step energy ΔE as $\Delta E_{\text{steric}} \uparrow \Delta E_{\text{bare}}$. At the upper terrace of the S_{\parallel}^* step, the steric repulsion is approximately the same as in the flat surface. Therefore, in this case $\Delta E(S_{\parallel}^*) \approx \Delta E_{\text{bare}}(S_{\parallel}^*) \approx 0.8$ eV. On the other hand, the difference $\Delta E(S_{\parallel}^*) \approx \Delta E(S_{\perp}^*) \approx 1.0$ eV/a reflects approximately $\Delta E_{\text{steric}}(S_{\perp}^*)$ (since the steric repulsion is absent at the S_{\perp}^* edge, row *a* in Fig. 2-a!). This $\Delta E_{\text{steric}}(S_{\perp}^*) \approx 1.0$ eV/a translates into 1.0 eV/at at the step, which can be compared to the energy gain ≈ 0.18 eV/at! due to the rotation of dihydrides on flat surfaces¹⁰ -which is a *partial* steric energy gain minus the elastic cost of the rotation!. When the *full* steric energy is removed from the S_{\perp}^* step, its formation energy becomes negative. -ii! Note in Fig. 2-b! that at the center of the terrace, the rotation of the dihydrides is parted into two regions. This division creates extra space that also

Oshiyama, we find that in the $(2\bar{3}1)$ phase all steps have positive formation energies, which implies that the flat surface is stable against step formation in the $(2\bar{3}1)$ phase. But our results suggest that the same might not be true for the $(3\bar{3}1)$ phase for H chemicals potentials close to the transition to the $(1\bar{3}1)$ phase.

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