Kim and Chelikowsky Reply: In their Comment [1] on our recent Letter [2], Harper et al. suggest that our *ab initio* calculation for the As vacancy ($V_{As}$) on the GaAs (110) surface, and other existing *ab initio* calculations [3,4], are in *qualitative* disagreement with the experimental scanning tunneling microscopy (STM) images [5]. Moreover, they argue that an atomic geometry, obtained by tight-binding molecular dynamics, is more reasonable than the minimum-energy geometry determined by *ab initio* calculations [5]. We believe their conclusions are unwarranted. In particular, Harper et al. do not present any theoretical support for their claims such as a theoretical STM image or an accurate estimate for the structural energies involved.

The central point of our Letter is the prediction of a geometry for the surface $V_{As}$ which includes an inward relaxation, not an outward relaxation, of surface Ga ions adjacent to the $V_{As}$. The Comment points to apparent discrepancies between the theoretical STM image and the experimental one. For example, Harper et al. suggest there is no lateral shift of the Ga atoms adjacent to the vacancy. In making this assertion, one must assume that there is no tip-surface interaction and that the atomic geometry is in registry with the electronic wave functions. Neither assumption is likely to be correct.

The question regarding the lateral shift of the two surface Ga images centers on technical differences between the simulated and the measured STM. Within the Tersoff-Hamann theory [6], which we have used to generate theoretical STM images, an infinitely sharp STM tip is considered whereas the experiment corresponds to finite sized tip. A convolution of the theoretical STM image with the tip function is required for a detailed comparison. However, the *main features* such as the pronounced tunneling into the two surface Ga sites next to the $V_{As}$ are expected to be reproduced correctly. We illustrate this in Fig. 1 where the tip height profile along [110] through the two surface Ga neighbors is shown. Aside from the expected discrepancies such as the larger theoretical corrugation (due to the infinitely sharp tip in simulations), theory and experiment agree very well. The secondary bright spots originate from the second nearest neighbor As ions [2], not from the third nearest neighbor Ga ions as proposed by Harper et al. [1]. We believe the apparent discrepancy between theory and experiment with respect to these spots is due to the existence of a strain field which is not fully released within the supercell geometry.

We have examined in some detail a geometry with outward relaxed surface Ga neighbors (as proposed by the authors of the Comment). This geometry is extremely unstable showing $\sim 1.4$ eV larger defect formation energy compared with the *ab initio* geometry. The two outward-relaxed surface Ga neighbors are subject to very large quantum forces ($\sim 1$ eV/Å).

We note in the tight-binding model, the stable charge state of $V_{As}$ on the $p$-type GaAs (110) surface was determined to be (+2). This strongly disagrees with recent experimental work [7]. In fact, one can show that the (+2) charge state can never be realized for $V_{As}$ on the GaAs (110) surface [2]. In contrast, the *ab initio* calculations [2,4] predict the stable charge state to be (+1) which agrees with experiment.

We believe any interpretation of STM images should be based on rigorous theoretical approaches, such as *ab initio* pseudopotential calculations, which can yield STM images and accurate structural energies.

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