Radny *et al.* Reply: In response to the points raised in the above Comment [1], we have carried out extensive calculations of the Ge(001)$c4 \times 2$ clean surface using a slab containing 8, 10, and 12 Ge layers, respectively. These calculations have again been performed using the VASP code. While the reconstruction of the surface was found to be little different to that obtained in our original calculations using 6 Ge layers, the electronic structure was found to vary significantly with the number of layers, in agreement with the findings of Yan *et al*. The band structure obtained using the primitive unit cell and 12 Ge layers is shown in Fig. 1. Comparison with the corresponding band structures for 6, 8, and 10 layers shows that the dispersion of the bands at the top of the valence band (TVB) along the Γ-J, Γ-K_1, Γ-J', and Γ-K_2 symmetry directions is strongly layer dependent, with the dispersion along Γ-J actually reversing in sign. The nature of some of the states near the TVB, and the size of the predicted energy gap, are also layer dependent. All of these conclusions are consistent with the findings of Yan *et al*.

The distribution of the different surface states and surface resonances for the 12 layer slab is also shown in Fig. 1. This shows, as stated by Yan *et al.*, that the true back bond surface states occur $\sim$0.5 eV below the Fermi Energy (E_F) near the Γ point, and that these states become surface resonances as one approaches the J point.

To further clarify the nature of the states, we have determined the spatial variation of their charge distribution normal to the surface, by integrating the charge density for each state over x and y. The highest occupied state at the J point has an exponentially decaying envelope confirming it is a surface resonance. The corresponding state for our original 6 layer slab, which lies at the TVB, is also a surface resonance. Moreover, this state has the bulk of its charge distributed along the bonds between the first and second, and third and fourth, layer atoms, analogous to the state shown in Fig. 4(c) of our original Letter [2]. Thus, the highest occupied states for 6 layers are indeed back bond surface resonances as we claimed.

We agree with Yan *et al.*, however, that this is no longer the case when the number of layers is increased to 10 or 12. For these thicker slabs, the states at the TVB occur near the Γ point (see Fig. 1) and are really bulk states. Near the surface, however, these states are characterized by a charge distribution arising from back bonds between the first layer (dimer) and second layer atoms. They thus reproduce charge density plots analogous to those shown in Figs. 4(a) and 4(b) of our original Letter, and low-bias simulated STM images dominated by double-lobed features on the up-Ge atoms, in agreement with experiment. It is thus these states that give the low-bias Ge(001) images their distinctly different appearance to low-bias Si(001) images, where the pi state dominates at the Fermi energy.

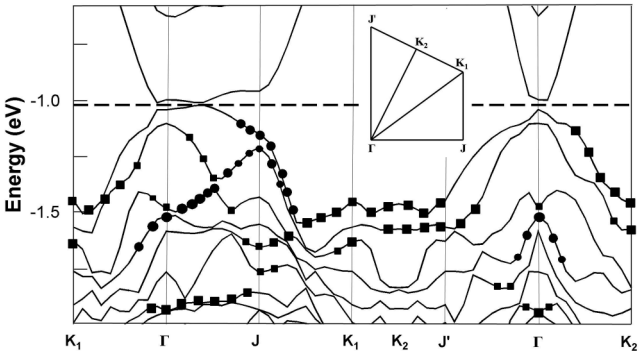

FIG. 1. Electronic structure of the Ge(001)$c4 \times 2$ clean surface for the primitive surface unit cell and a periodic slab containing 12 layers, with the top of the valence band (TVB) indicated by the dashed horizontal line. The irreducible part of the Surface Brillouin zone is shown in the inset. The surface states and resonances are indicated by symbols, with the size of the symbol indicating the degree of surface localization: ● back bond, ■ dangling bond.

The change in the electronic structure with increasing number of layers also affects the relationship between the back bond and dangling bond surface states. In our original Letter, we concluded that the states at the TVB for Ge(001)$c4 \times 2$ were back bond states, and that the dangling bond states were $\sim$0.35 eV below E_F. While this is correct for the 6 layer slab, the 12 layer calculations yield a very different result, as shown in Fig. 1. We observe that in this latter case, some of the dangling bond states occur quite close to the TVB, and are essentially degenerate with the highest-lying back bond surface resonances. It thus follows that the distinctions that we were drawing regarding the energy distributions of the back bond and dangling bond surface states of the Si(001)$c4 \times 2$ and Ge(001)$c4 \times 2$ surfaces in the vicinity of E_F are no longer so clear cut.

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