Ciraci and Batra Reply: We reported[1] that K adsorbed on Si(001)-(2×1) at $\theta=1$ (one K per two surface Si) donates valence electrons to the empty surface-state band, and forms a strong ionic bond. The otherwise semiconducting substrate surface is thus transformed into a metallic one. The surface metallicity arises from partial occupancy of the dangling-bond (DB) band, and not from the K chain. The energetics[1,2] of the K-Si system ($\simeq 2.5$ eV binding energy) also argues against the metallization of K. These conclusions have been confirmed by recent experiments.[2-4]

In the preceding Comment,[5] Kasowski and Tsai (KT) have asserted that K does not form an ionic bond with Si. Since the ultraviolet photoemission spectrum of Cs+Si(111)-(2×1) is different from that of K+Si(001)-(2×1), and electron-energy-loss spectroscopy excitations at $\simeq 1.7$ eV have also been observed on clean Si(001)-(2×1), these experiments do not directly support the KT model calculations. The remaining arguments—density of states and charge of the K overlayer—are based on an arbitrary charge partitioning, and thus are not conclusive. Their scheme assigns the high charge density of the Si surface to the K overlayer. Since the lowest-value contour of clean Si surface in Fig. 1(b) is already larger than the maximum charge density of the unsupported K chain in Fig. 1(d), this leads to an artificial transfer of charge from Si to *less electronegative* K. As a matter of fact, the amount of charge between a plane from 1.06 Å above the surface to infinity is larger than one electron even for the clean surface with half-filled DB band.

The local-density approximation underestimates the structural parameters[6] of K. However, we would like to prove that the bonding is strongly ionic even for a larger value of $d_{(\text{Si-K})}$. To this end we show the self-consistent-field charge distribution for a measured[7] value of $d_{(\text{Si-K})}=6$ a.u. (3.2 Å). Plots of valence-charge-density difference, i.e., $\rho\{\text{K+Si}\}-\rho\{\text{Si}\}$ in Fig. 1, unambiguously show the DB as the origin of surface metallization, and not the metallic K chain. Because of the disproportionate scale of their axes (see KT's Fig. 1), they[5] have apparently missed the fine structure in the charge-density plots, such as the double hump of the DB, and hence their Fig. 1 shows disparity with our Fig. 1(e). Finally, Hartree-Fock calculations[8] have also found strong ionic bonding for this system.

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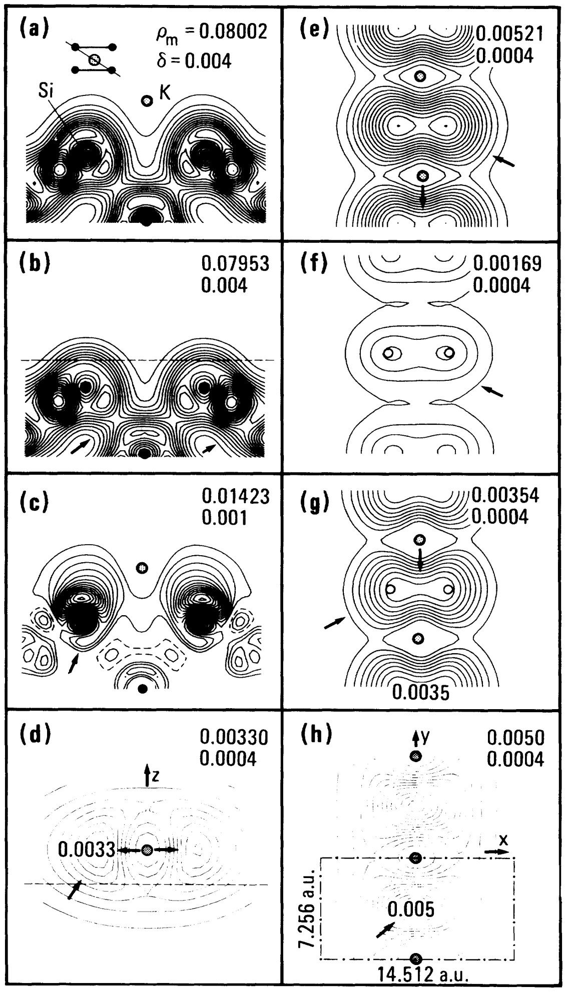

FIG. 1. Contours of total charge density. First column: in a vertical plane passing through K and two nearest surface Si [as shown in the inset of (a)]. (a) K+Si(001)-(2×1) with $d_{(\text{Si-K})}=6$ a.u.; (b) clean Si(001)-(2×1); (c) difference plot of (a) and (b); (d) unsupported, metallic K chain in registry with K on Si(001)-(2×1). Second column [(e)-(h) in the same order as the first column]: in the plane of K overlayer 4.2 a.u. above the surface silicon. ρ_m, maximum value of charge; δ, contour spacing. Dashed line in (b) indicates the lateral plane 1.06 Å above the surface.

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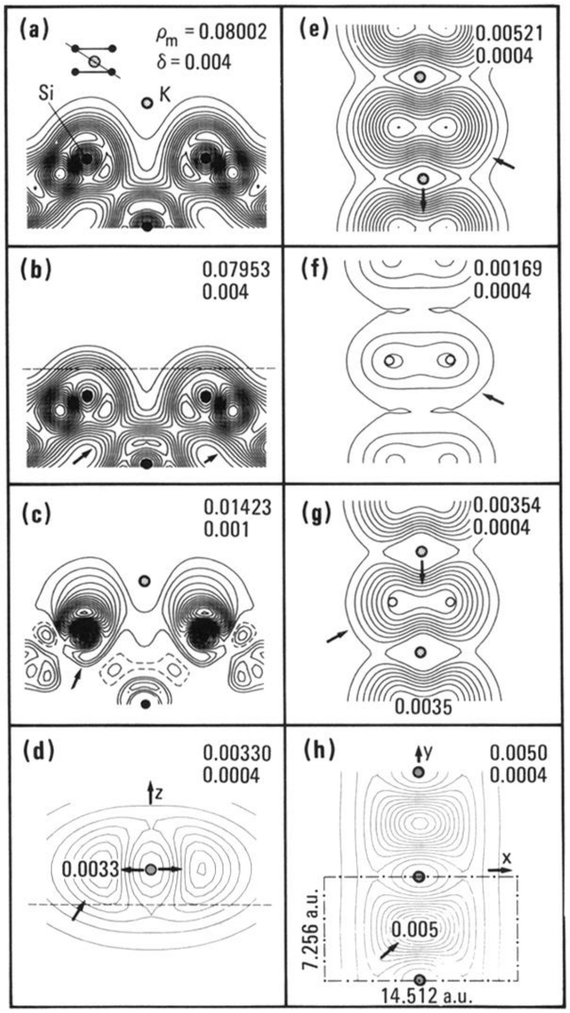

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