

Comment on "Novel Electronic Properties of a Potassium Overlayer on Si(001)-(2×1)"

Angle-resolved electron-energy-loss spectroscopy measurements indicate "that K chains adsorbed onto Si(001)-(2×1) are in the nature of a one-dimensional metal."¹⁻³

The above theoretical and experimental point of view is not consistent with a recent self-consistent, geometry-optimized, total-energy pseudopotential calculation⁴ for a K overlayer on Si(001)-(2×1) surface. It is found that the metal-insulator transition has its origin in active dangling bonds and not in the conventional Mott transition with a bond length of only 2.59 Å.

Total-energy calculations using the pseudofunction method⁵ support the earlier theory² and experiments^{1,3} indicating metallic chains of K. The K atom sits at the center of the sixfold hollow site, between two parallel dimer bonds with a K-Si bond length of 3.30 Å. A plot of bonding charge in the K plane (see Fig. 1) indicates a metallic chain in the (110) direction. The total charge from a plane 1.06 Å above the Si atoms to infinity is 1.15 electrons, indicating metallic chains.

The computed total density of states and K-layer density of states [Fig. 2(a)] have peaks which are very similar to those observed via ultraviolet photoemission spec-

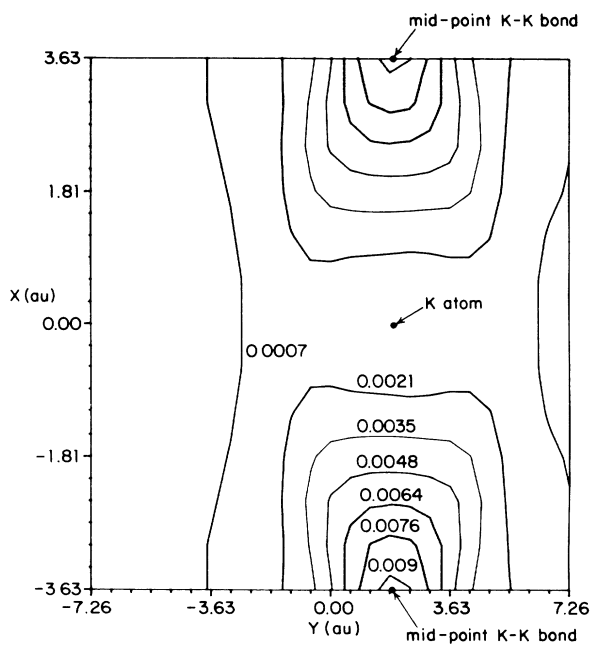


FIG. 1. Contours of nonspherical charge density for a plane passing through the K atoms which are 7.25 a.u. apart in the x direction.

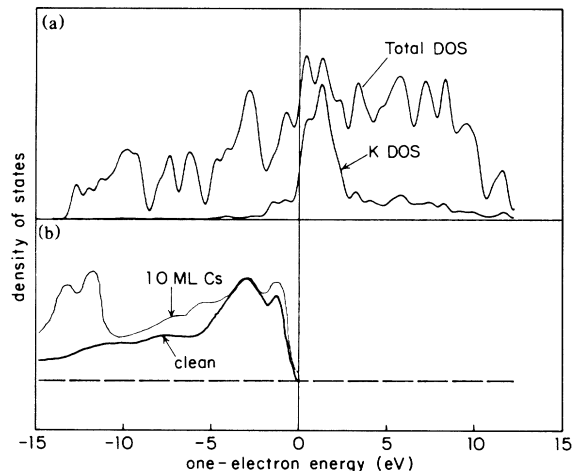


FIG. 2. (a) Calculated density of states (DOS) for K on Si and K-layer local density of states. (b) Ultraviolet photoemission spectroscopy (UPS) spectrum for Cs on Si(111)-(2×1).

troscopy⁶ for Cs on Si(111) [see Fig. 2(b)]. Similar structure would be expected for K on Si.

Recent surface extended x-ray-absorption fine-structure measurements⁶ indicate a bond length of 3.14 Å.

R. V. Kasowski

Experimental Station
Central Research and Development Department
E.I. du Pont de Nemours and Company
Wilmington, Delaware 19898

M.-H. Tsai

Department of Physics
University of Notre Dame
Notre Dame, Indiana 46556

Received 20 January 1987

PACS numbers: 71.30.+h, 71.45.Gm, 73.90.+f

¹Tetsuya Aruga, Hiroshi Tochiwara, and Yoshitada Murata, *Phys. Rev. Lett.* **53**, 372 (1984).

²Masaru Tsukada, Hiroshi Ishida, and Nobuyuki Shima, *Phys. Rev. Lett.* **53**, 376 (1984).

³Hiroshi Tochiwara and Yoshitada Murata, *J. Phys. Soc. Jpn.* **51**, 2920 (1982).

⁴S. Ciraci and Inder P. Batra, *Phys. Rev. Lett.* **56**, 877 (1986).

⁵R. V. Kasowski, M.-H. Tsai, T. N. Rhodin, and D. D. Chamblis, *Phys. Rev. B* **34**, 2656 (1986).

⁶T. Kendelewicz, P. Soukiassian, R. S. List, J. C. Woicik, P. Pianetta, I. Lindau, and W. E. Spicer, *Phys. Rev. B* (to be published).