calization or spectral features. The methods of AH, SCLC, and PP all provide such information directly, and have demonstrated ability to produce accurate bulk band structures. We believe that these results provide a much firmer basis than BC's for relating surface geometry and spectroscopic data.

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Commentary on the Effect of Relaxation on the Electronic-Energy-Level Structure of the Si(111) Surface

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In the preceding Comment, Appelbaum and Hamann have compared our self-consistent-field, $X\alpha$, scattered-wave cluster model calculations with some other surface calculations for Si(111). In this paper we briefly review their and our semi-infinite slab calculations with a view to a further understanding of the effect of surface relaxation. We offer a rebuttal to some of the comments made by Appelbaum and Hamann regarding our calculations.

In a recent Letter,[1] we reported the electronic level structures for ideal, relaxed, and reconstructed (2×1) Si(111) surfaces, all calculated self-consistently by the scattered-wave (SCF-$X\alpha$-SW) cluster model.[2,3] For the most part, our findings were in good agreement with the results known earlier.[4-6] Our calculations went beyond and made some new predictions about the reconstructed surface. For example, we predicted the absence of a superlattice energy gap for the Haneman model[7] of the (2×1) reconstructed surface. Several calculations have subsequently confirmed independently[8-10] that one needs to extend Haneman's model to obtain the experimentally observed[11] energy gap.

Appelbaum and Hamann (AH) have rightly pointed out in the preceding paper[12] that, for the relaxed case, their calculation does not fully agree with ours. Specifically, AH's calculation predicted that the S_2 surface states do not appear unless the surface relaxes inwards by at least 0.18 Å. We found[1] charge transfer and energy shifts upon relaxation which agreed reasonably well with AH's, but we did not find surface relaxation to be the origin of S_2. Based on our experience with many types of cluster calculations we do not accept the views expressed by AH[12] suggesting that this discrepancy necessarily arises from shortcomings of the cluster model calculations.[1] Since it does not seem to be possible to resolve this issue experimentally, we recognize that the debate is somewhat academic in nature.

It has been amply demonstrated in the literature[13-18] that cluster model calculations provide physically realistic results. The essential features of complex multiatomic problems are usually revealed by suitably chosen cluster models. The primary reason for the success of the cluster models is that the electronic properties of many solids are determined principally by the local atomic arrangement. The cluster method takes advantage of this circumstance and provides useful information on bulk as well as surface electronic structure. Therefore, we fully expect the method to be successful for the Si(111) surface.

AH have indicated[12] that the saturation of those parts of the surface not under study by H atoms is not justified. The saturation of the dangling bonds with H atoms to minimize end effects has been justified with a criterion[15] different from ours, and has been successful in the past.[15,16] Using the same procedure, we find that the calculated total density of states for the Si(111) surface agrees well with the experimental findings.[4]

In addition, we have recently studied the Si(100) surface[19] using the SCF-$X\alpha$-SW cluster model[2,3] Our computed total density of states for the ideal Si(100) surface, which is shown in Fig. 1, agrees quite well with those given by tight-binding calculations.[20] The orbital character of the surface states A and B also agrees with the results given by other calculations.[6,21] Thus, we are able to demonstrate once again that the saturation of bulk Si bonds with H atoms is a very reasonable scheme.

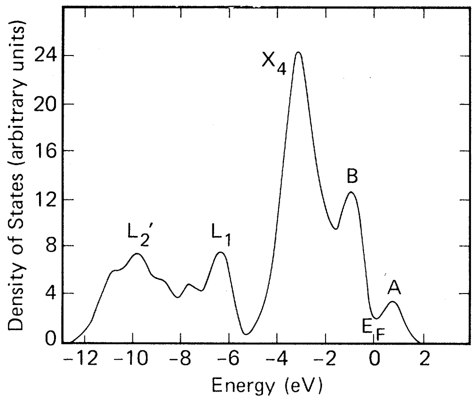

FIG. 1. Total density of states for the ideal Si(100) surface. The unoccupied surface band, A, primarily consists of the p_y-type orbitals. The occupied surface band, B, consists of p_z-type orbitals. (The z axis is perpendicular to the surface.)

AH have stated[12] that our clusters are too small to permit systematic identification of surface states. It is certainly true that if the cluster size is too small, a systematic interpretation of the results is very difficult. It is precisely for this reason that we modeled the Si(111) surface with clusters of widely different sizes. We also studied the sensitivity of our results to various calculational parameters. From these numerous computations, we were able to draw conclusions[1] which were cluster-size independent. We have also been able to conclude[19] that for the Si(100) surface, the cluster $Si_{18}H_{22}$ is adequate. This is comparable in size to the clusters we had used earlier[1] for studying the Si(111) surface. It should be noted that our model clusters for Si(100) and Si(111) have different point-group symmetries. Since our clusters are able to represent properly different surfaces, we can rule out the suggestion[12] by AH that the back-bonding surface states may be an artifact of the model.

AH claim[12] that the muffin-tin approximation made in our calculations is producing large errors. We do not believe that the muffin-tin approximation can produce large errors when the calculation is carried out to full self-consistency. This should be evident from our calculation[1] where we are getting a total valence bandwidth of 13 eV for the Si(111) surface. This compares favorably with other available results.[4-10,20,22]

It is misleading to quote (as AH do[12]) the work by Kane[23] and by Williams and Morgan[24] in this context. These authors[23,24] carried out *non-self-consistent* band-structure calculations using *ad hoc* crystal potentials, while our calculations were fully self-consistent. It is possible that they[23,24] would have found considerably smaller errors (relative to experiment) if they had carried out their calculations self-consistently. Furthermore, our calculations were performed within the framework of the overlapping atomic spheres model[25] as opposed to the touching sphere model. This has the effect of further reducing the muffin-tin region and improves the physical realism of our calculations. The theoretical justification for the overlapping atomic sphere model has been provided by Herman, Williams, and Johnson.[25] Therefore, we believe that the muffin-tin approximation as employed in our calculations is well justified.

Of course our calculations, like other calculations, are based on various approximations. We believe that the disagreements among various calculations for the relaxed case might well arise from the inexact nature of the potentials used. This possible deficiency is clearly not limited to our cluster model calculations. Therefore, let us examine whether the potential used[5,12] by AH is sufficiently realistic to warrant conclusions as firms as they wish to draw.

(1) The most serious criticism of the method used[5,12] by AH is that their potential is constructed[26] in terms of four adjustable parameters not subject to self-consistent improvement. As pointed out by Chelikowsky and Cohen,[27] "the meaning of achieving a self-consistent potential with respect to an adjustable core potential is not clear, as any total potential can be made self-consistent to some type of core potential." Thus the calculation by AH can be characterized in all fairness as semiempirical. Our calculations, on the other hand, take into account all the electrons and are fully self-consistent.

(2) AH have used[5,12] two-wave-vector point sampling in their "self-consistency" scheme. It has been argued by Cunningham[28] "that the two-point sample may be too small to give accurate results," especially when the surface-state band is only partially filled, as is the case for ideal and relaxed Si(111) surfaces.

(3) Finally, for the relaxed structure for the Si(111) surface, AH construct their potential using procedures which are not unique.[5] They introduce a hypothetical crystal with every sixth (111) plane displaced. One would hope that these potentials would assume a more realistic form through self-consistency. However, since AH's calculation[5,12] does not appear to be fully self-consistent in the traditional sense, we cannot judge how realistic their final potential is.

In view of these shortcomings of AH's work,[5,12] we cannot accept their assertions that back-bonding surface states are a consequence of relaxation. AH model potentials[5,12] are too approximate and the self-consistency too ill-defined to give us a high degree of confidence in their conclusion that the origin of back-bonding surface states is relaxation. It is also not clear how sensitive their results[5,12] are to the location of the arbitrarily chosen "matching plane"[5] for Si(111), where surface states have been found to be localized in the third atomic layer.[9] Furthermore, AH have carried out their calculations for a limted number of k_s points. It is possible that back-bonding surface states are in fact localized for the ideal structure at points other than those few investigated by them. We feel that a definite resolution of the disagreement cannot be made at the present time. Whether or not such a moot point is worth resolving is left up to the judgment of other workers in the field.

A critical reading of the present manuscript by Dr. F. Herman is gratefully appreciated.

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CONNECTION BETWEEN CHARGE-DENSITY WAVES AND SUPERCONDUCTIVITY IN $NbSe_2$. R. C. Morris [Phys. Rev. Lett. 34, 1164 (1975)].

From page 1164, column 1, line 20, citation to the following reference was omitted, after "... negative coefficient." H. N. S. Lee, H. McKinzie, D. S. Tannhauser, and A. Wold, J. Appl. Phys. 40, 602 (1969).

In addition, reference should have been made in the Letter to the following earlier work on the Hall effect in $NbSe_2$ having iodine impurities. D. J. Huntley and F. R. Frindt, Can. J. Phys. 52, 861 (1974).

FRICTION COEFFICIENT OF AN ABSORBED H ATOM ON A METAL SURFACE. Klaus-Peter Bohnen, Miguel Kiwi, and Harry Suhl [Phys. Rev. Lett. 34, 1512 (1975)].

Nourtier and A. Blandin (private communication) have drawn the authors' attention to a misleading statement in the above paper. After Eq. (15) it is stated that spherical symmetry of the mixing potential is sufficient to ensure vanishing of the coefficients ν^α. In fact the ν^α then vanish only in the bulk, and not for motion near the surface, especially normal to the surface. A publication by Nourtier and Blandin is in preparation.

SELF-CONSISTENT PSEUDOPOTENTIAL CALCULATION FOR A METAL-SEMICONDUCTOR INTERFACE. Steven G. Louie and Marvin L. Cohen [Phys. Rev. Lett. 35, 866 (1975)].

The discussion in this paper relating our results to Inkson's work is somewhat misleading. Our intention was (1) to state that the pinning of the Fermi level in the semiconductor gap can be explained by our gap states without relying on Inkson's arguments related to merging bands; and (2) to comment on the inappropriateness of a band picture for small distances. However, because of our use of the Slater statistical exchange, we cannot comment directly on the properties which may result from the dynamic and nonlocal exchange integral as used by Inkson.