

ERRATA

tion, which describes the situation with the crystal in its ground state and no core hole, is also the final-state Hamiltonian for emission. Initial- and final-state *pictures* refer to the ways in which transition matrix elements are calculated. In the initial-state picture both states entering the matrix element are eigenstates of the initial-state Hamiltonian, while in the final-state picture matrix elements are taken between eigenstates of both the initial- and final-state Hamiltonians. Thus, for example, the initial-state picture for emission describes the matrix element taken between core and valence eigenstates both in the presence of a core hole, while the final-state picture for emission describes the matrix element taken between a core eigenstate in the presence of a core hole and a valence eigenstate in the absence of core hole.

To remain in accord with these definitions, the words "initial-state Hamiltonian" used throughout the text to describe the eigenstates Ψ_{core} and Ψ_{val} should be replaced by "initial-state Hamiltonian for absorption," i.e., the Hamiltonian in the absence of a core hole.

Furthermore, the following corrections are necessary on page 3070:

(a) At the end of the sentence immediately following Eq. (2.1b') it should read: "... , the correct Hamiltonians to use should be those appropriate for the final-state picture.⁵⁵⁻⁵⁷"

(b) In column 2, line 18 it should read: "We have, therefore, chosen to use the initial-state picture for absorption, Eq. (2.1a'), and the final-state picture for emission, Eq. (2.1b)."

Erratum: Surfaces of real metals by the variational self-consistent method [Phys. Rev. B 17, 2595 (1978)]

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In Table VII the values given for the LDA surface energies of the bcc (110) faces of some alkali metals were erroneously copied from values calculated for hypothetical fcc (111) faces. The correct bcc (110) values are 358, 227, 137, and 108 ergs/cm² for Li, Na, K, and Rb, respectively. In Table IX the surface energy σ for Mg hcp (0001), including the wave-vector correction $\Delta\sigma_{xc}$, should be 618 and 614 ergs/cm² by the perturbational and variational self-consistent method, respectively. We thank Dr. Norton Lang for pointing out some discrepancies due to these copying errors (which do not propagate into other parts of the paper). Note that surface energies of magnitude greater than 750 ergs/cm² have been rounded to the nearest 5 ergs/cm²; they agree with the ones given in our Letter [Phys. Rev. Lett. 37, 1286 (1976)], where surface energies of magnitude greater than 200 ergs/cm² were rounded.

In Sec. I we stated that the variational self-consistent method gives an upper bound to the surface energy for a given energy functional. Rigorously, the method provides an upper bound to the *total* energy. This implies an upper bound on the surface energy when the effect of bulk density variations $n(\vec{r}) - \bar{n}$ on the bulk binding energy is zero.