

to the observed phase transition. The work reported here provides that evidence by demonstrating that the computed electronic energies and wave functions actually do lead to an isomorphic phase transition at unit cell volumes very near those experimentally associated with the isomorphic phase transition of Cs.

The energy bands found for Cs resemble so closely those reported by Yamashita and Asano [10] that it is unnecessary to present them here. The cohesive energy per atom calculated from these bands and from the corresponding wave functions is shown in Fig. 1a as a function of the volume per primitive unit cell (per atom) for both the fcc and the bcc structures. The calculated equilibrium cohesive energy for the bcc phase (-0.061 Ry/atom) is in good agreement with the experimental value of -0.062 Ry/atom reported by Gschneider [12], and the calculated equilibrium unit-cell volume, 780 cubic atomic units (Bohr radii), agrees well with the 745 cubic atomic units determined experimentally by Barrett [13]. The computed energy curves predict the fcc phase to be the O K equilibrium phase, in contradiction to the experimental results. However, the computed energy difference between the fcc and bcc phases at the equilibrium volume is small and

may well be due to use of the muffin-tin approximation. (Since the same (fcc) phase prevails on both sides of the high-pressure isomorphic transition, the errors due to this approximation should be nearly identical for the two phases involved and should thus be unimportant in the investigation of that transition.)

It is significant that the $X\alpha$ calculations do so well for the cohesive energy, because the model does not include any explicit estimate of the correlation energy. Slater [1] has suggested that the local ($X\alpha$) exchange approximation itself includes certain features of correlation. For example, it leads to the correct separated-atom limit for the one-electron eigenvalues and the total energy, and it treats excited one-electron states in a more desirable fashion than is done with the virtual states in the Hartree-Fock method. (For instance, the undesirable and non-physical vanishing of the free-electron-gas density of states at the Fermi energy, which is obtained in the Hartree-Fock approximations, is eliminated by the local, averaged exchange of the $X\alpha$ method.) It may thus be that the $X\alpha$ approximation includes certain of those features of the correlation correction which are most crucial to binding, even though it does not explicitly include any correlation term. (For accurate cohesive energies, it is only necessary to duplicate the variation of the correlation energy as the atoms coalesce into the solid or molecule, not to