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and Kendrich (Ref. 2).
~4The first-order phase transition and critical behavior
of MnO are also explained well by the 2D

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16.5

16.5

17.4

17.4

(c)

(d)

FIG. 3. Charge-density contours for the ln'„orbital
of Si2. Labels as in Fig. 1 except for the contour steps in (a) and (b) which are 5 electrons per cell. (a) From Ref. 8, (c) from Ref. 1.

es the magnitude of the valence charge in the bond region: from 83.4, 33.2, 16.5, and 59.5 electrons per cell for 10&, 1o„, 1~„, and 2cr„ in the unor-thogonalized limit, to 97, 35.9, 17.4, and 64.2 electrons per cell after orthogonalization, com-pared to the all-electron results of 73, 36, 19, and 55, respectively. The maximum orbital den-sities obtained with the nonlocal first-principles pseudopotentials 76.8, 36, 19.2, and 53.7 com-pare well with the 36,

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play an essential role for the occupied levels of
Si (while excited states might differ by a volt or
more) provided the local form is spatially suffi-
ciently localized. "'4'

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In this study we have discussed general charac-teristic features of projected (pseudopotential) orbitals which for many problems of interest give physical insight and, if intepreted correctly, can be used in place of real orbitals. Furthermore, recently proposed pseudopotentials constructed either from first principles or by explicitly fit-ting to all-electron atomic wave functions'4 are found to yield improved energies and charge den-sities for molecules and soli in close agree-
ment with all-electron results.
%e thank D. R. Hamann and G. A. Baraff for helpful discussions. This work was supported in part by the Division of Basic Energy Sciences, U. S. Department of Energy, and by National Sci-
ence Foundation under Grant No. DMR76-20647-AOI.

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