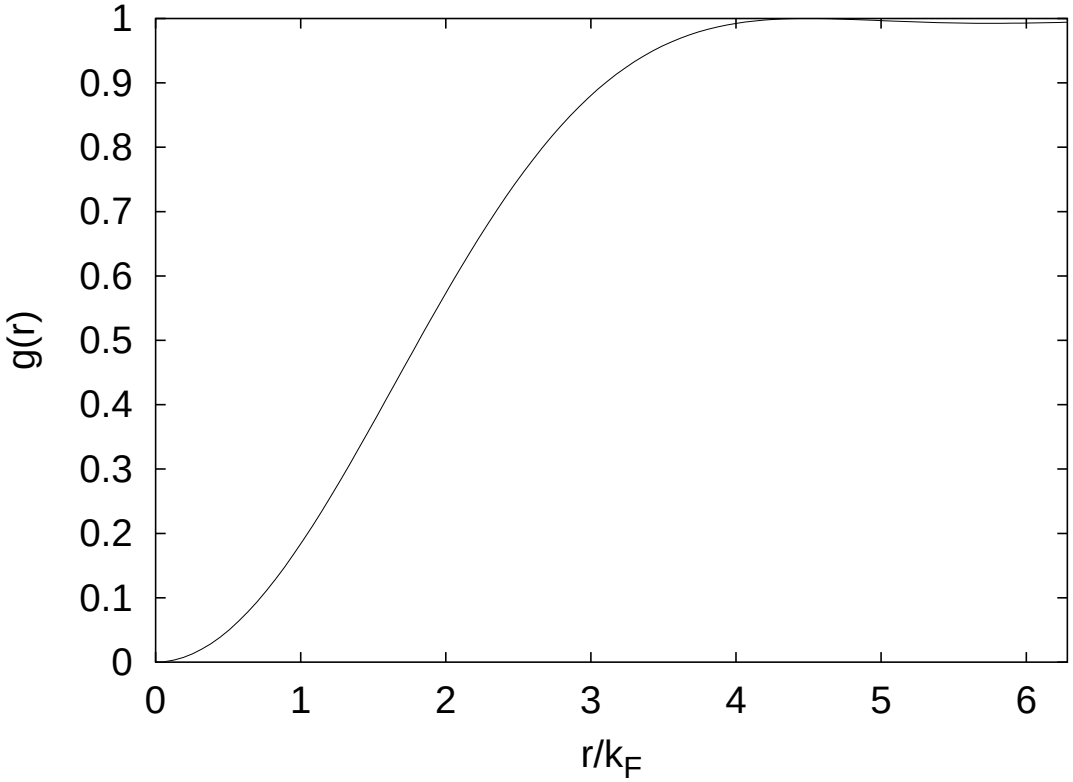
exchange hole (HF)

unpolarized homogeneous electron gas

$$k_F = (3\pi^2 n)^{1/3}$$

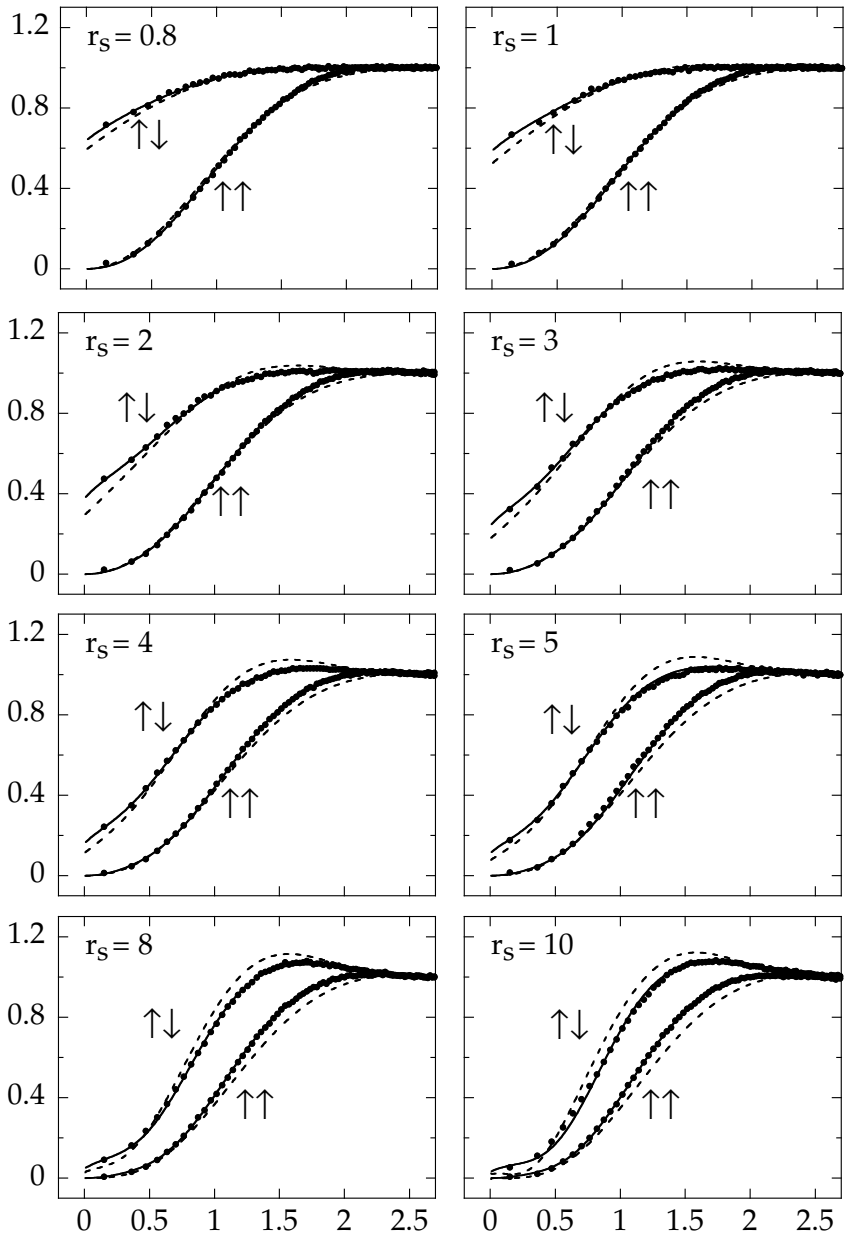
$$g_x(r) = 1 - \left[\frac{3}{(k_F r)^3}\{\sin(k_F r) - k_F r \cos(k_F r)\}\right]^2$$



exchange-correlation hole (QMC)

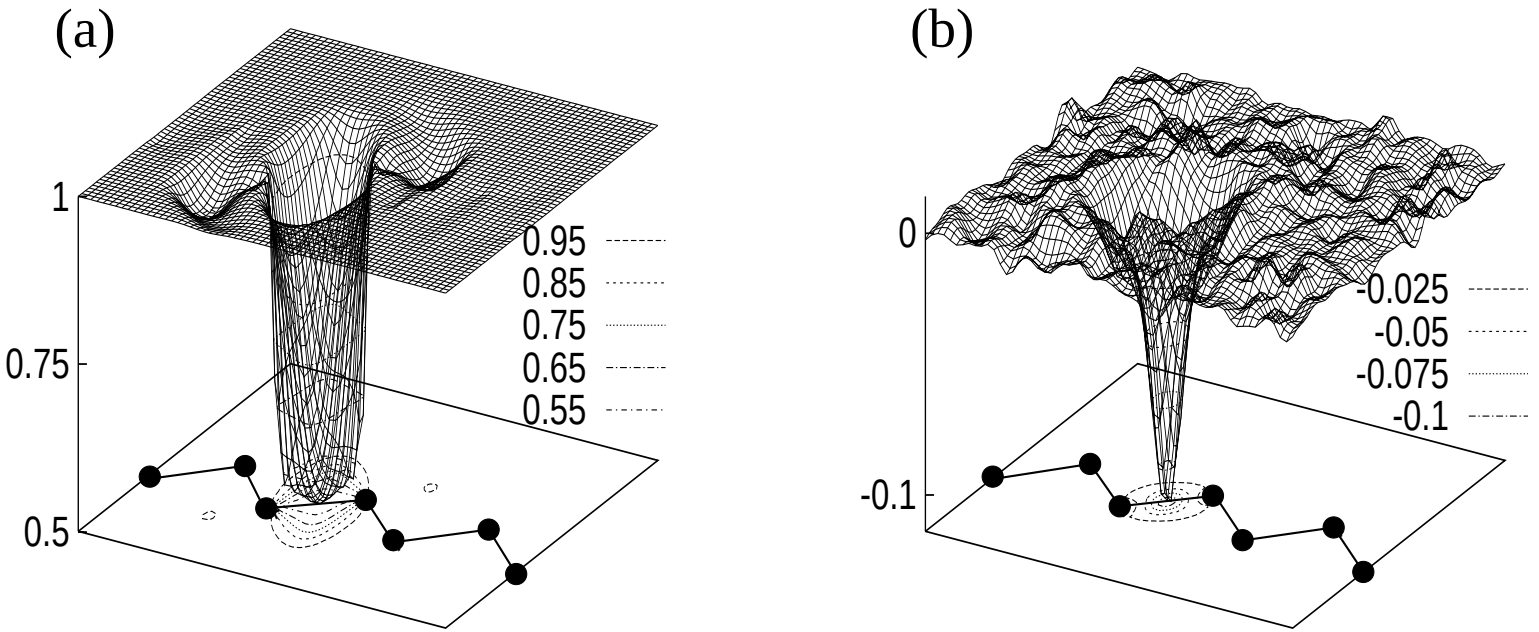
unpolarized homogeneous electron gas

$g_{xc}^{\sigma\sigma'}(r/r_s)$ with $r_s = (3/4\pi n)^{1/3}$



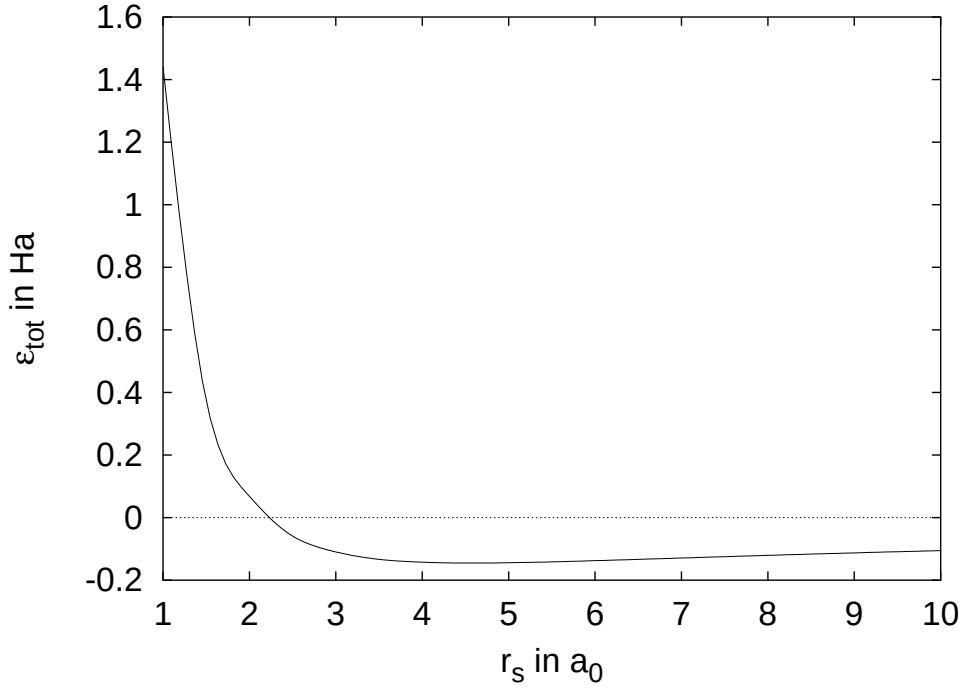
G. Ortiz, M. Harris, P. Ballone, Phys. Rev. Lett. **82**, 5317 (1999)
P. Gori-Giorgi, F. Sacchetti, G.B. Bachelet, Phys. Rev. B **61**, 7353 (2000)

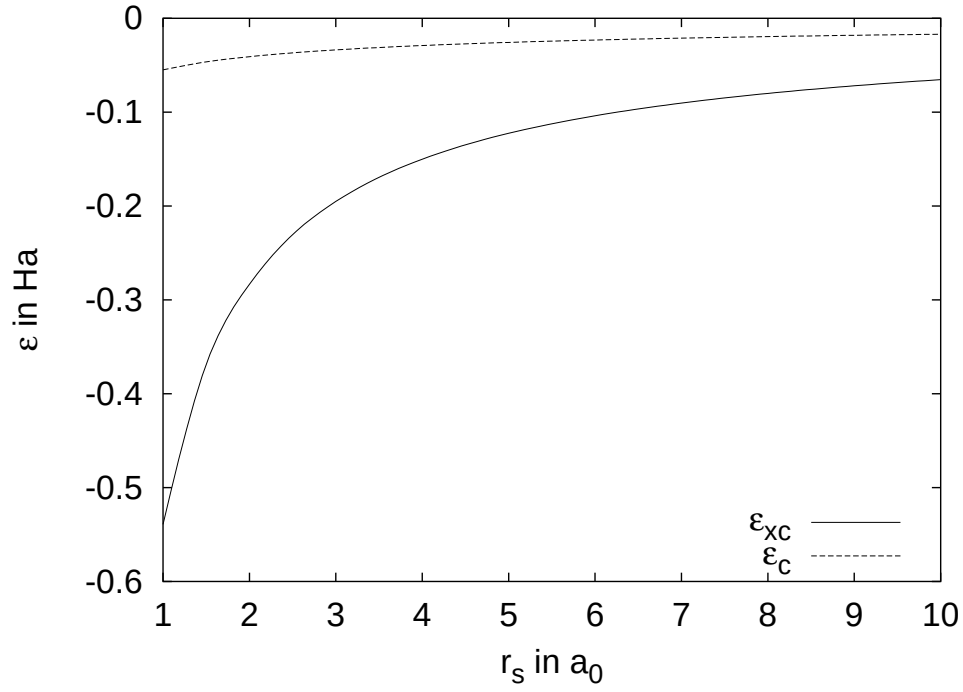
exchange and correlation hole (VMC) for electron at bond center in Si



R.Q. Hood, M.Y. Chou, A.J. Williamson, G. Rajagopal, R.J. Needs, W.M.C. Foulkes, Phys. Rev. B **57**, 8972 (1998)

homogeneous electron gas (QMC)





D.M. Ceperley, B.J. Alder, Phys. Rev. Lett. **45**, 566 (1980)

Charge density for C_{60}

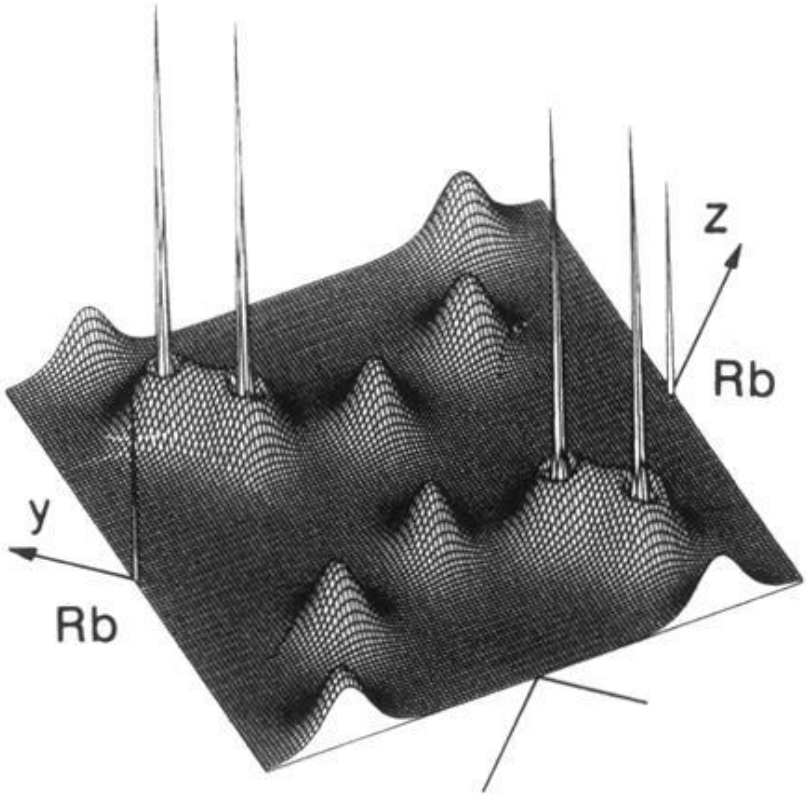
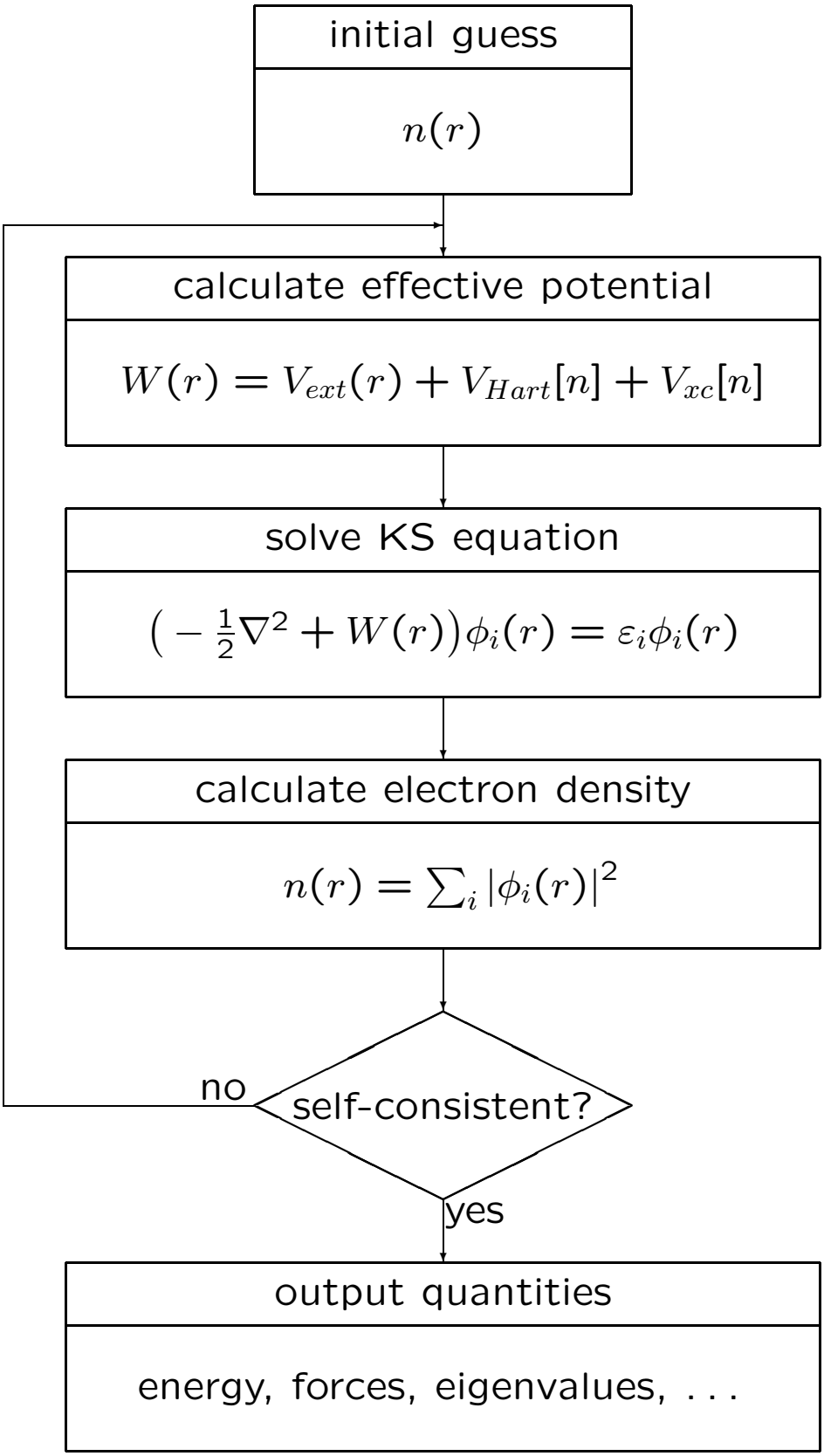


FIG. 12. Valence charge-density in the yz plane (see Fig. 2) for RbC_{60} in the fcc unidirectional structure. The plane passes through the Rb octahedral sites and, for each of two neighboring molecules, it contains a top hexagon edge and passes between two contact atoms plus the midpoint of another top hexagon edge. The Rb $5s$ electron is seen to be transferred to the C_{60} molecule.

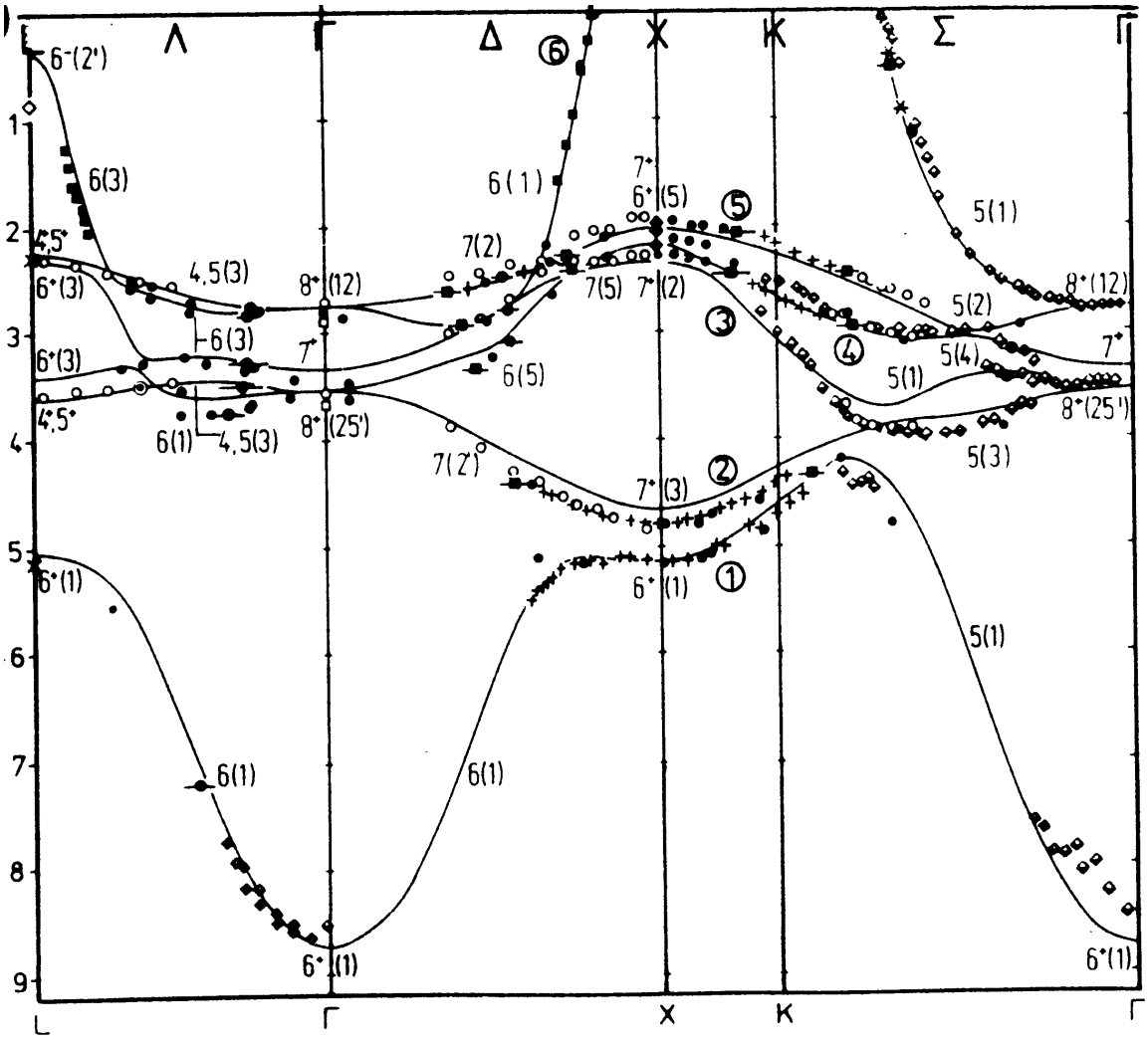
S. Satpathy, V.P. Antropov, O.K. Andersen, O. Jepsen,
O. Gunnarsson, A.I. Liechtenstein, Phys. Rev. B **46**, 1773 (1992)

Solving the KS equations



Band structure of copper

angular resolved photoemission (ARPES)
APW calculation



P. Thiry et al., Phys. Rev. Lett. **43**, 82 (1979)

G.A. Burdick, Phys. Rev. **129**, 138 (1963)

Fermi surfaces

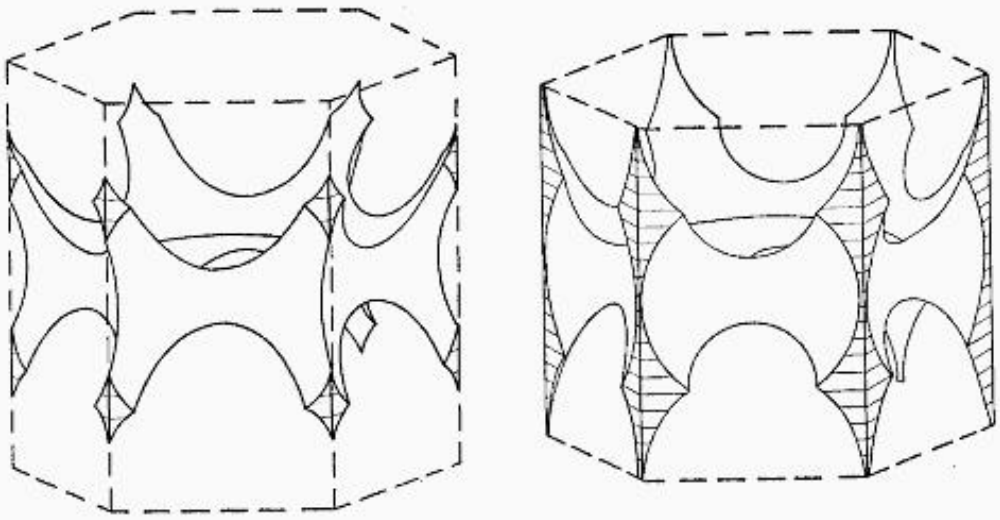


FIG. 4. Fermi surface in the combined first and second bands of divalent hexagonal-close-packed metals according to the single-OPW approximation. The figure on the left corresponds to an ideal c/a ratio of 1.633; that on the right to a c/a ratio of 1.862, roughly that of cadmium.

W.A. Harrison, Phys. Rev. **118**, 1190 (1960)