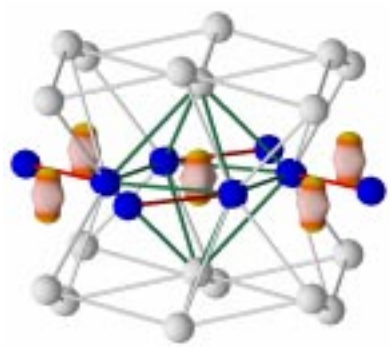
Electron densities in Cs-V and Si-VI

U. Schwarz*, O. Jepsen, and K. Syassen

Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany

Cesium-V

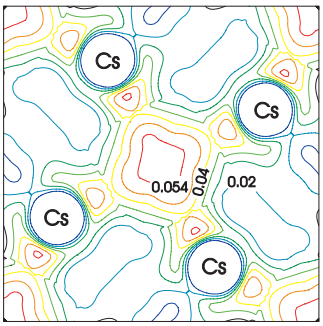
3D contour and ELF



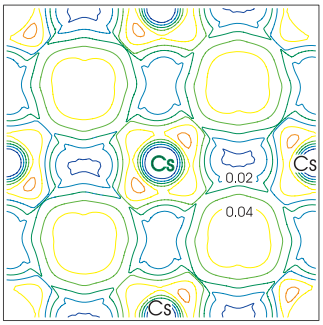
Electron density maxima and attractors of high ELF values are found within the centers of one type of octahedra at x = 0. The arrangement of these regions reveals strong similarities to a framework of condensed octahedral clusters with two electrons per polyhedron [A. Savin et al., Angew. Chem. Int. Ed. **36**, 1808 (1997)].

2D electron density contours

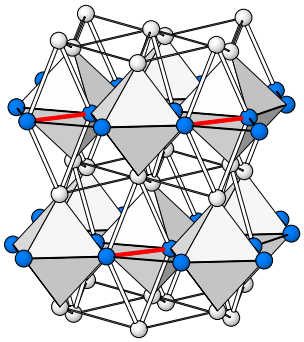
(100) plane, x=0

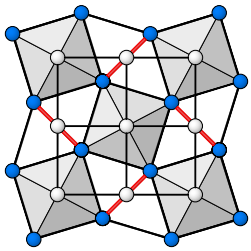


(100) plane, x=0.25



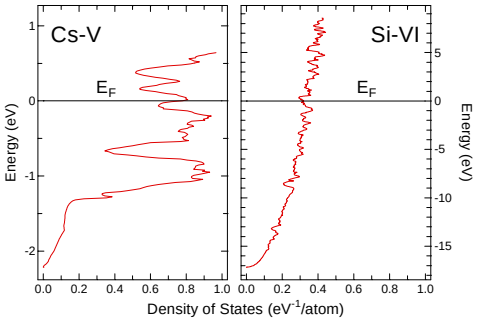
Cmca (Z=16)





The orthorhombic crystal structure (a/c = 1.69, b/c = 1.005) is formed by layers of corner-sharing distorted octahedra. The atoms occupy two different Wyckoff positions [8f (0,y,z; blue), 8d (x,0,0; white)] with 11- and 10-fold coordination, respectively. The structure can be viewed as distorted fcc. With respect to coordination numbers it is intermediate between tetragonal Cs-IV (CN 8) or hexagonal primitive Si-V (CN 8) and ideal close-packing (CN 12).

Density of States

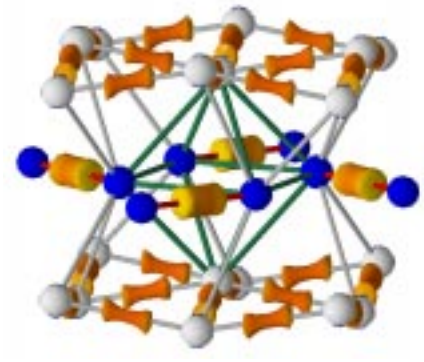


The occupied bands in silicon have mainly sp-character whereas in cesium d-bands dominate below the Fermi level.

Band structure calculations based on the Stuttgart tight-binding LMTO code [G. Krier et al., MPI-FKF Stuttgart 1998].

Silicon-VI

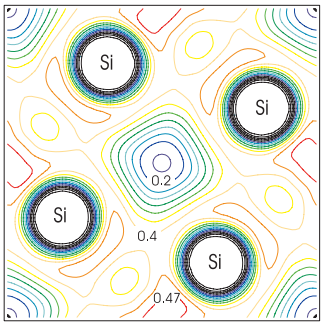
3D contour and ELF



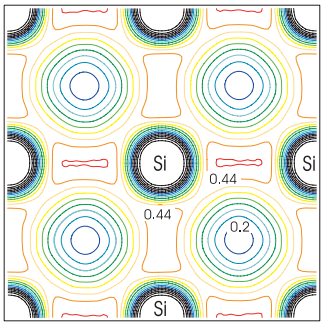
The electron density of Si-VI shows remarkable differences with respect to that of Cs-V. Charge maxima and regions of high ELF values indicate covalent bonding in both types of layers. For x = 0, the formation of Si_2-dumbbells is already indicated by electron density. At x ≈ 0.25, four-bonded silicon atoms form puckered nets.

2D electron density contours

(100) plane, x = 0



(100) plane, x = 0.25



* Present address: Max-Planck-Institut für Chemische Physik fester Stoffe, D-01257 Dresden, Germany.