# Chpt. 11: Other methods

Self-consistency

Valence bands

$U_K \sim Ry$

Very short wavelength  /// many components

1. Solve w/in a cell (Wigner & Seitz)

$$\psi(r) = e^{-ik\cdot R}\psi(r+R)$$

$$\hat{n}\cdot\nabla\psi = -e^{-ik\cdot R}\hat{n}(r+R)\nabla\psi(r+R)$$

Spherical inside

expand $Y_{lm}$

keep finite terms

2. Muffin-tin  $\phi_{k,\varepsilon}$ interstit.

solve middle

match

APW

ung. ave

KKR Green FNT.

Integ. form. S.E. still keep finite #

3. OPW ~~~ coverg. much faster

nearly F.E. fits

4. Pseudopotential