

in the middle of Chapter 5

## Bandstructure of the electrons

Kohn-Sham eigenvalues for periodic solids (crystals) are classified

by 2 quantum numbers:  $\vec{k}$ ,  $n$  band index  
 $\vec{k}$   $\equiv$  wave vector

$\vec{k} \equiv e^{i\vec{k}\cdot\vec{R}_I}$  = eigenvalue of

translation operator:  $T_{\vec{R}_I}$

with  $\{\vec{R}_I\} \equiv$  Bravais lattice

Two examples of bandstructure

