

in the middle of Chapter 5

Bands structure of the electrons

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

by 2 quantum numbers: \vec{k} , n band index

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

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

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

Two examples of band structure

