Exercise 11

Molecular and Materials Modelling

May 16, 2019

1 Band structure calculation

The goal of this exercise is to compute the bandstructure of a liner chain of atoms in a tight binding framework. In the first part, you will build the computational tool and in the second part, you will use the developed tool to understand intriguing conceptual aspects of bandstructure.

Task 1 Make use of your knowledge of Bloch's theorem introduced in the lecture, and the hints given in the markdown cells in the notebook, to complete the missing lines in the Exercise-11.ipynb.

Task 2 Test your code by computing the bandstructure of a linear chain of atoms with a single atom/orbital per unit cell. Use an energy of 0.1 eV for the orbital and an hopping term of -0.2 eV. You should obtain a cos-like dispersion.

Task 3 Consider a liner chain with a single atom per unit cell having two orbitals with energies of -0.25 eV and -0.1 eV and an hopping term of 0.1 and -0.1 eV respectively. Comment on the bands that you obtain. Can you associate the simulated case to a example presented in the lecture?

Task 4 Consider the 1D atomic dimer chain introduced in the lecture. Try to obtain the plots in the lecture-notes and explain your choice of input parameters that you used to reproduce the bands.