

Learning with the tight-binding model

Before considering real materials with properties calculated within the density functional theory, we will focus on the tight-binding model. The advantage of this approach is two-fold. First, the effective models contain a much smaller number of parameters compared to the real crystal structures, thus representing a simpler task to start with. Second, a large amount of data can be generated in a relatively short time, which is necessary for machine learning algorithms.

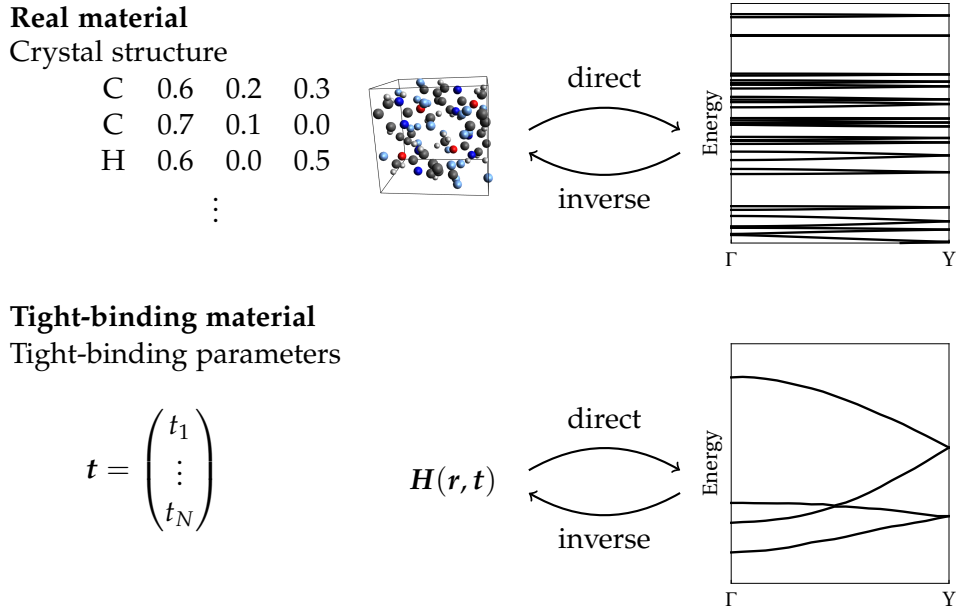


Figure 4.1: Schematic comparison of a real material and a generic tight-binding material.