Übungen zur

Computational Nanoscience

– Blatt 7 –

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Aufgabe 1) Tight-Binding Model

Calculate a tight-binding energy spectrum for the 2-dimensional cubic lattice with nearest-neighbor hopping t_1 and next-nearest hopping t_2 as well as for the triangular lattice with nearest-neighbor hopping t. Is there is some special case where these two band structures can be similar?

Aufgabe 2) Density of States

Find the density of states (DOS) for the 1-dimensional tight-binding model with nearest-neighbor hopping t.

Aufgabe 3) Wannier orbitals

Proof that the Wannier orbitals are orthogonal for different bands (n) and different lattice sites $\vec{R}$:

$$W_n(\vec{r} - \vec{R}) = \frac{1}{N_k} \sum_{\vec{k}} e^{-i\vec{k} \cdot \vec{R}} \Psi_n^{\vec{k}}(\vec{r})$$

where the $\Psi_n^{\vec{k}}(\vec{r})$ are the solution of effective Schrödinger equation in crystal.