Übungen zur

Computational Nanoscience

– Blatt 6 –

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Aufgabe 1) Bravais Lattice

Show that the Graphene (2d-honeycomb) lattice is not a Bravais lattice and find the corresponding basis with translations. How many atoms in unit cell has the Buckyball (Fulleren) superconductor K_3C_{60} with the FCC lattice.

Aufgabe 2) Wigner-Seitz-Cell

Proof that volume of the Wigner-Setz cell multiplied with volume of the Brillouine zone in 3 dimension is equal to $(2\pi)^3$.

Aufgabe 3) Plane-wave basis

Proof that for any reciprocal vectors $\vec{G}$ and $\vec{G}'$

$$\frac{1}{V}\int_V d^3r e^{-i\vec{G}\vec{r}} e^{i\vec{G}'\vec{r}} = \delta_{\vec{G}\vec{G}'}$$