

Übungen zur  
CiS-Computational Physics

– Blatt 9 –

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**Aufgabe 1) DOS for TB-model**

Calculate Density of States (DOS) for 2-dim. 3 band TB-model of High-temperature superconductors (HTSC) and 3-dim. 1 band TB model using MindLab-software.

**Aufgabe 2) Electronic structure of Si**

Calculate band structure of Si using MindLab-software. How large is the bandgap?

**Aufgabe 3) Magnetism of Iron**

Calculate magnetic band structure of BCC and FCC Fe. Obtain the magnetic moment of BCC iron (Experiment:  $2.2 \mu_B$ ).