Exercises

Computational Materials Science

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Sheet 1

Exercise 1: Density functional theory

Use the Wien2K code to calculate the ground state energy, bandstructure and the partial densities of state of TiC.

The steps to this end will be discussed in the exercise hour.

You can also follow the QuickStart section of the user guide available at http://www.wien2k.at/reg_user/textbooks

Explore your own paths, e.g., calculating other materials, other physical quantities, compare LAPW and APW+lo results, convergence w.r.t. many parameters, compare LDA and GGA ...