GETTING INSIGHT INTO CONDENSED MATTER BY AB INITIO CALCULATIONS

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The main message of this lecture is that experimental research into the properties of condensed matter can benefit a lot from using the increasingly accurate information that can be delivered by *ab initio* calculations. By "*ab initio* calculations", we mean the search for solutions to the basic quantummechanical equations for solids, using as few approximations as possible and avoiding all experimental input. The basics behind Density Functional Theory – the most widely used *ab initio* approach in condensed matter physics – will be outlined. The interplay between theory and experiment will be illustrated by a few selected examples.

Some of the issues discussed in the present lecture can be found in:

Density Functional Theory and the family of (L)APW-methods: a step-by-step introduction
S. Cottenier
Editor: Instituut voor Kern- en Stralingsfysica, K.U.Leuven, Belgium
ISBN 90-807215-1-4 , 2002, 70 p.
Freely available at http://www.wien2k.at/reg_user/textbooks.

Ab initio calculation of hyperfine interaction parameters: recent evolutions, recent examples
S. Cottenier, V. Vanhoof, D. Torumba, V. Bellini, M. Çakmak, M. Rots
(To appear in *Hyperfine Interactions* in 2005 – proceedings of HFI-2004 in Bonn)