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Calculation of technologically important aspects of magnetism: anisotropy, critical temperatures and spin dependent transport

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Abstract

Magnetic materials, where the moments arising from the electron spins are ordered, have many potential applications of technological relevance. For instance, in recent years the focus has been on spintronics, a future technology where not only the electron's charge but also its spin will be utilized. In this presentation we will deal with a few of these applications from a microscopic theoretical view. The discussion is based on calculations of the electronic structure often within (spin) density functional methods.

A large magnetic anisotropy, the fact that there are considerable energy differences between different magnetization directions, has considerable importance for e.g. magnetic storage and permanent magnet applications. We will discuss here how to calculate this quantity, which is exemplified by both a bulk system and a layered material, and the calculational accuracy and the method's predictability.

One example of spin dependent transport is the so-called spin transfer torque, the fact that a current through a magnetic layer can rotate its magnetization. We will review its physical origin and present some recent calculations on naturally magnetic layered materials, so-called helical spin density waves.

A crucial quantity for applications of the various spectacular magnetic effects is the Curie temperature, the temperature above which the magnetic order disappears. Many systems are limited by low Curie temperatures. A route to calculations of this quantity is described, and with the help of a few calculations we try to generalize what is needed to achieve significant magnetic ordering temperatures.

