MAGNETIC MATERIALS MODELING FROM FIRST PRINCIPLES

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As early as the 1960s, physics students could learn that: [...] *we should expect that it is a combination of electrical forces and quantum-mechanical effects that will determine the detailed structure of materials in bulk, and, therefore, their properties* (R. P. Feynman, Feynman Lectures on Physics). The modern first-principles calculations are a practical form of realizing these expectations. The advances in computer performance observed over the past few decades and the accompanying development of dedicated computing codes make it possible to achieve both high precision of the calculated results and the determination of many physical parameters previously unavailable.

In this presentation I will discuss the basic classification of magnetic materials, their properties, and aspects of spin-polarized first-principles calculations. I will introduce the relationships between real materials, their theoretical models and the methods used to perform the calculations. Furthermore, I will discuss the three layers of magnetic material models, which are crystal, electronic, and magnetic structure. As part of the presentation, I will review aspects of modeling permanent magnets and determining their three key intrinsic parameters which are magnetization, Curie temperature and magnetocrystalline anisotropy [1, 2]. I will cover issues of preparing structural models for modeling antiferromagnets and I will also discuss ways to model chemical disorder and interstitial doping. Finally, I will proceed from bulk material models to models of layered systems used in spintronic applications [3]. I will discuss aspects of preparing layered heterostructures and the capabilities and limitations of selected computational codes in modeling magnetic layered systems. The original results presented here were obtained mainly using the full-potential local-orbital minimum-basis code FPLO [4, 5].

References

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