

Oponentský posudek disertační práce

Saleem Ayaz Khan: Electronic structure calculations as an aid to study structure and magnetism of layered materials

The main topic of the work is the question of the applicability of electronic structure calculations to calculate several important properties of FePt, foremost the magnetocrystalline anisotropy (MCA) and atomic moments. This topic is of high importance, since obtaining an optimal value of MCA is a crucial ingredient in different kinds of magnetic storage memories. Generally the work contributes to the field of spintronics, which has a great application potential. Ab initio calculations are now widely used to predict material properties and it is thus important to have an assessment of its validity presented in this work.

The work employs density functional theory within the local density approximation. Two possible basis schemes are used: the full potential linear augmented plane wave method and the Korringa-Kohn-Rostocker method. Ab initio calculation methods always require some approximations and here I find the employed approximations to be appropriately chosen. The applicant has also verified the convergence with respect to possible numerical parameters of the methods, for example the k-point mesh density. Disorder has been described either by the coherent potential approximation (CPA) or special quasirandom structures of various sizes. Relativistic effects crucial for the MCA has been included either using the complete approach based on Dirac equation or by a perturbative inclusion of spin-orbit interaction. These were compared to each other. These are state-of-art methods and there is no method generally better than those.

The work provides MCA energy for stoichiometric FePt and its 50:50 alloy. It examines this energy as a function of the spin-orbit interaction magnitude. The effect of different LDA parametrizations, relativity treatments, and application of the magnetic force theorem is examined. Employing various supercells composed of disordered FePt the variation of atomic momentum due to the surrounding atoms in the alloy has been calculated and compared to the momentum provided from CPA. Overall the thesis contributes to the field as an original and comprehensive study of the accuracy of different numerical ab initio methods related to magnetism and foremost the magnetocrystalline anisotropy.

The work is well organized, it is carefully split into chapters and sections. I see no formal errors and only a very low number of grammatical mistakes.

The work is supported by an impressively long list of publications, 40 in total, which is high above the requirements for a Phd defense. These papers are mostly published in standard condensed matter physics journals, I could not find any in a more prestigious journal.

Some points are not sufficiently explained and more information about them is desirable:

Why has the MCA not been calculated for the disordered system? What do you expect to happen in that case with MCA compared to the ordered FePt?

Why do you think LSDA overestimates the MCA energy of FePt, while for many materials it underestimates MCA? How good agreement is achieved for orbital momentum as compared to experiments?

What is the reason for the inapplicability of CPA to study core level broadening? Is it true also for valence state broadening, can CPA be extended to include core level broadening?

Based on the above listed findings I recommend the thesis for defense.

V Praze 3.7.2017

RNDr. Karel Carva, Ph.D.



Oponentský posudek

na dizertační práci Saleema Khana

„Electronic structure calculations as an aid to study structure and magnetism of layered materials“

Reviewer's report

on the doctoral dissertation of Saleem Khan

„Electronic structure calculations as an aid to study structure and magnetism of layered materials“

Layered materials form an important class of new materials that are being explored for potential use in many aspects of technology. Indeed, it was probably the molecular beam epitaxy with its ability to produce well-defined multilayers that started a revolution in materials engineering. Even though the field of materials engineering is mainly technological and experimental, theoretical studies are in a great need here because they may essentially contribute to understanding the underlying mechanisms and principles. The topic of the dissertation is thus clearly important.

The author focuses mainly on magnetism of layered compounds and used FePt as an archetypal material. The advantage of focusing on FePt is that this is a well-established material with a lot of theoretical and experimental results so there is a solid basis to built on and a lot of stuff to compare. The danger of this focus is that it might be difficult to contribute with really useful original results because the manifold research that has been done so far. The author avoids this danger by focusing on those aspects of magnetism that are still only incompletely understood: the magnetic anisotropy and the interplay between magnetism and disorder. The results thus may contribute not only to research on FePt itself but also to understanding of the above mentioned topics in general.

Throughout the study the author relies on first-principles quantum-mechanical framework which proved to be useful in this respect. The author combines two quite different methods for electronic structure calculations: the multiple-scattering Korring-Kohn-Rostoker Green's function method (KKR-GF) and the full-potential linearized augmented plane waves method (FLAPW). This combination of different methods is certainly valuable. A careful comparison of results of KKR-GF and FLAPW method for such a sensitive quantity as the magnetocrystalline anisotropy energy is very useful on itself. Moreover, it demonstrates that the author must have mastered use of both methods which may prove very useful in his possible future research. It should be stressed, nevertheless, that the asset of the work is not only methodological. The dissertation presents two important physical conclusions: (i) The magnetocrystalline anisotropy of FePt cannot be quantitatively described unless many-body effects beyond the local density approximation (LDA) or the generalized-gradient approximation (GGA) are taken into account and (ii) neglect of the Madelung contribution to the Coulombic potential in the coherent potential approximation (CPA) affects significantly the average magnetic moment of disordered FePt. It would be certainly interesting to know to what degree these conclusions could be generalized to other systems. So my main question to the author is whether he tried similar calculations for other systems? If yes, what were the results and to what degree are they compatible with the results for FePt? If not, I wonder how general the conclusions presented in the thesis? For which compounds can be expect similar results?

Further, I have some minor points. The author pays a lot of attention to comparison of the magnetocrystalline anisotropy energy (MAE) evaluated by subtracting total energies and via the magnetic force theorem. What are practical implications of the comparison? Would author recommend use of the magnetic force theorem or not? And what about calculations of the MAE using the DFT+U formalism? Can we expect a significant improvement over LDA and GGA calculations? Finally, I would like to ask about structural relaxations. The author used FLAPW for this. Could the same research be done using the KKR-GF formalism? What about the pseudopotential framework which is commonly used for structure optimization: could be expect identical results?

Judging the dissertation formally, some phrases could be formulated in a more eloquent way but generally the style is quite good. Purely technically, I think the text in some figures is sometimes quite small and not easy to read (in particular, in figures 6.12-6.15). Sometimes there are misprints in the axes titles (figure 6.17). As a whole, the plots are nevertheless illustrative and mostly clear.

The publication record of the author is surely satisfactory, he is co-author of quite a lot of research papers and in several of them he is the first author. I believe that the results which form the core of the submitted thesis will be used and appreciated by the research community.

To conclude, I recommend the dissertation to be defended.

Praha, 19. June 2017



RNDr. Jiří Vackář, CSc.