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Reviewer's report on the doctoral thesis of Agnieszka Lidia Kozub

(Charles University):

„Electronic structure and magnetic properties of the materials with strong electron-electron correlations"

During the last decades it has become clear that electronic correlations in solids lead to the emergence of novel, unexpected phenomena. These correlation effects are not only of interest for fundamental research but also have a great potential for technological applications. In particular, correlation effects in systems with reduced dimensionality offer previously unexpected opportunities for the construction of materials with desirable functionalities and the development of entirely new devices. A big role in these developments plays a calculational design by means of the first principle approaches such as density functional theory in combination with dynamical mean field theory. From this part of the thesis it is not clear in what extend A. Kozub was also involved in the methodological and code development.

The main aim of the thesis of A. Kozub is to investigate electronic structure of strongly correlated materials by means of DFT++ methods. In particular, two classes of materials are investigated: a) magnetic impurities in bulk copper and graphene, b) novel Np-based compounds.

Thesis starts with short introduction, where author brings her research into broad context of correlated physics. Following two chapters are devoted to the density functional theory and DFT++ methods which serves as a formal basis for the investigations presented here. Main emphasis is given the various flavors of the mean field approaches. These chapters are very well written and it is clear that A. Kozub internalized whole theoretical methodology on a very high level.

Main results of this thesis are summarized in the chapter 3 and 4 and both chapters are based on the four published scientific manuscripts. All manuscripts are published in a high level journals and in two of them A. Kozub is a first author. In the chapter 3 A. Kozub in a detail discuss magnetic inpurities, in particular Co, diluted in the copper host. All calculations are done within the framework of LAPW in combination with exact diagonalisation DMFT solver. I believe that in addition

University of West Bohemia
New Technologies – Research Centre
Univerzitní 8, 306 14 Plzeň, Czech Republic

Phone: (+420) 377 63 4771

E-mail: jminar@ntc.zcu.cz

to the results presented here, the detailed comparison to the continuous-time QMC in an important result. Even-though it is technical aspect of the study, it is very interesting to the DMFT community. Last part of the Chapter 3 is devoted to the rare-earth adatoms on graphene. Here author discuss effects of the spin-orbit coupling and correlations onto the properties of graphene and predicts ground state of the Nd-adatom.

Last Chapter is devoted to the novel Np-based compounds. This chapter is based on the results which where obtained in a close collaboration with the experimental colleagues in Gdansk. Here A. Kozub focus on the 1-2-7 group of Np-based compounds which shows novel magnetic properties which as author nicely shows are related with local ordering on Np atoms. Studies here are based on the DFT+U method and author shows an crucial role of the spin orbit coupling on the magnetic properties of these compounds. In addition to the theoretical calculations, A. Kozub discuss in a detail various experimental results obtained for these componds. This is surely very important add on of this work. In this chapter, however I miss discussions or even results from the DMFT method. Discussions about possible dynamical effects beyond LDA+U in these compounds would be very helpful to understand correlations in these materials. At the end of the thesis, A. Kozub summarizes in results of the whole thesis. Conclusions are clearly written, however I do miss some more general outlook of work presented here, predictions found in the thesis and possible suggestions for new experimental as well as theoretical work.

To summarize, submitted work of A. Kozub is very well written and discuss many important aspects of the electronic correlations. All together, A. Kozub published 8 manuscripts, what is surely very good number. Submitted content-rich thesis undoubtedly reflects her great competence also proofs her achieved scientific independence. Accordingly, I suggest the submitted thesis to be accepted and the dissertation of A. Kozub to be defended.

Plzen, 11.1.2018, Doc. Dr. Jan Minar

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New Technologies – Research Centre
Univerzitní 8, 306 14 Plzeň, Czech Republic

Phone: (+420) 377 63 4771

E-mail: jminar@ntc.zcu.cz