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Review of the Ph.D. thesis "*Electronic structure and magnetic properties of the materials with strong electron-electron correlation*" by Agnieszka Lidia Kozub, Charles Univerisity in Prague, Faculty of Mathematics and Physics, Department of condensed matter physics supervised by Ing. A. B. Shick, CSc., DSc., Institute of Physics, Czech Academy of Sciences of the Czech Republic.

The thesis contains ca. 80 pages . Theoretical chapters amount to first 40 ones, second half is devoted to the own first-principles calculations and measurements. The results deal with three different problems, Cu impurity in Co (Kondo effect); Sm and Nd adatoms on graphene; Np-based heavy fermion systems, where the author took also part in the experimental investigations that is rarely seen and definitively deepers her condensed matter knowledge.

The theoretical part treats the standard single electron framework of density functional theory (DFT) with brief description of the localization technique using fully localized limit and around the mean field approximation as two limiting cases. Next, more advanced treatment of electron-electron interactions as exact diagonalization follows. A great appreciation comes from the summary at the end of each chapter.

The outcome of the present study, the project one and four, resulted in publications in international review journals like Phys. Rev B (A. Kozub 2016), Conf. proceed. of WDS 2015, and Phys. Rev B (A. Hen 2015). This is considered as a very positive dissemination and as a proof of a actual topic in condensed matter physics and of interest among the community of strong correlations effects within solids.

Thesis is clearly written with minimal typos(see below), well structure and outlined and easy to read. Still there is a concern about the different features of underlying projects. Following questions could raise an higher interest about the investigated and related topics:

Questions and comments:

<u>Project: "Co in bulk Cu"</u>

1. Fig. 3.3 top panel, the Co-*d* DOS look like only t_{2g} component... Is it true? From the bottom panel there is a certain contribution of e_g states under E_F.

2. How did you adjust the Slater integrals values to which quantity?

3. How are (actually it covers all) chosen the parameters of U, J for all materials studied? Not much commented about it. Also the Rkmax and sampling of BZ seems to be rather small, especially for the spin-orbit calculations.

Project "Nd and Sm adatoms on grahene"

1. What is a justification of the exclusion of the f-states and bath orbitals in Sm on graphene as this leads to the correct results with both FLL and AMF?

2. Neither L, S or XAS is compared with experimental data?

3. Also of interest would be a comparison what the L, S, J are with repect to the pure Nd?

Project "Nd-based heavy fermions ($NpPt_2In_7$, Np_2Ni_{17},NpC)"

1. Was there any attempt to experimentally determine (e.g. XMCD measurement) the orbital and spin contributions of the Np-based compounds to be compared with the first-principle calculations?

2. Is there any intermediate scheme (a parameter) between FLL and AMF for Hubbard U technique?

Typos:

- p 13 1.1.2. theory theory
- p. 56 sucsesion
- p. 64 el. behavior localized (metallic bonds), itinerant (magnetic moments) → should be reverse

Conclusion: This Ph.D. thesis is a well approached combination of the advanced (Hubbard U technique of FLL and AMF limits and ED) first-principle calculations and experimental measurements that both aim to the determination of the magnetic properties (L,S, J, T_C, T_N etc.) in a complimentary manner. Therefore I recommend **this work** for the Ph.D.defense.

In Ostrava, Feb. 7th 2018

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