Institute of Physics of the ASCR, v.v.i.

Na Slovance 2, 182 21 Prague 8, Czech Republic

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Supervisor report on Ph.D. Thesis of Mgr. Maxim Tchaplianka.

Mgr. Maxim Tchaplianka started his PhD studies under my supervision in the Department of Condensed Matter Theory of the Institute of Physics of the ASCR in October 2018. The plan of his studies was two-fold: 1/ to learn and acquire practical experience of the electronic structure theory of realistic solid state materials making use of the density functional theory methods; 2/ to combine the modern numerical techniques for strongly correlated electrons with DFT, and to study the electronic structure and magnetism in complex solids and nanostructures.

Mgr. Maxim Tchaplianka showed good performance in accomplishing both topics. He learned DFT based packages VASP and in-house implementation of FLAPW, and applied it to FeHf-Sb alloys thermodynamic stability in terms of enthalpy of formation, and the magnetic anisotropy energy. These studies were motivated by the search of rare-earth-free magnetically hard materials for novel permanent magnets. The results were presented at the week of doctoral studies (WDS) at the Charles University, and published in a journal Crystals (2020).

Next, he learned how to solve the multi-orbital Quantum Impurity model for realistic materials making use of the finite temperature Lanczos method (Exact diagonalization). He developed and coded the efficient algorithm for constructing the finite bath from the DFT calculated hybridization function based on the Broyden-Fletcher-Goldfarb-Shanno minimization method. He applied it to study a Kondo behavior of Co adatom on a number of surfaces. Importantly, he showed by a direct numerical calculations that the spin-orbit coupling is crucial in formation of a singlet ground state for the adatom on the surface, contrary to the bulk where it plays practically no role. This work was done within the OPVV project "SOLID21‘‘. These results are published in a New Journal of Physics (2021) and Phys Rev. B (2022).

In a final part, he was actively imvolved in calculations of a number of U-based ferromagnetic U-Fe-Si alloys calculating their thermodynamic stability, the electronic and magnetic properties including the magnetic anisotropy energy making use of a combination of DFT with the many-body Exact diagonalization. These results are published in the Scientific Reports (2023).

In my opinion, he completed the scientific tasks very well, and demonstrated enthusiasm and devotion to the research. He showed himself as a hard-working and well organized individual. The quality and quantity of his research work is fully sufficient for obtaining the Ph.D degree.

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