The Ph.D thesis of Mr. Tchaplianka deals with the long-standing challenge of understanding the electronic structure and magnetic properties of strongly correlated materials. This is a very important topic, at the forefront of condensed matter physics, because the strong correlation often produces spectacular magnetic effects that are poorly understood.

The first two chapters of the thesis are devoted to a methodological survey. The first chapter explains the essentials of density functional theory, which is the workhorse of electronic structure theory. The second chapter deals with many-body methods, focusing on the exact diagonalization of a multi-orbital Anderson impurity model constructed from the results of the density functional theory calculation.

Chapters 3 and 4, which are the main chapters of the thesis, contain original research results obtained using the tools described in the first two chapters. Chapter 3 deals with Co impurities. In my opinion, the most important and original result of Chapter 3 is the identification of a Kondo singlet in the system of a Co atom adsorbed on a Cu(100) surface. This is a fundamental result because it explains experiment well, while also exposing the role of both spin-orbit coupling and the multi-orbital model in obtaining the correct result.

Chapter 4 deals with more complex systems, notably Fe- and U-containing compounds. Here, in my opinion the most important result is the prediction of $UFe_{10}Si_2$ as being potentially a magnetically hard material. This prediction is based on a calculated positive uniaxial magnetic anisotropy together with a negative enthalpy of formation.

To summarize, this thesis reports novel scientific results. It is well structured and clear, and I recommend its approval.