Title: Electronic structure and magnetic properties of materials with strong electron-electron correlations

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Abstract: In this thesis, we present several computational methods of studying magnetic materials, and apply them to several real materials. Density functional theory with exact diagonalization is used to investigate three materials which consist of a cobalt impurity coupled to a metallic substrate. The observables and spectral densities found in each case are presented. Next, FeHfSb and $UFe_{10}Si_2$ are investigated as potentially magnetically hard materials, via the calculation of their magnetocrystalline anisotropy and thermodynamic stability.

Keywords: density functional theory, Anderson impurity model, exact diagonalization, magnetic anisotropy, Kondo effect