In this thesis, we summarize the material-specific theories of strongly correlated systems and apply them to selected materials. We describe and apply the correlated band theory methods: the local density approximation plus Coulomb U, and the density functional theory plus exact diagonalization of single impurity Anderson model. First, we investigate the systems containing impurity atoms: cobalt impurity located in the bulk copper and samarium, and neodymium adatoms on the surface of graphene. We present the spectral densities and study the magnetism of those compounds. Afterwards, we analyze three Np-based compounds: $NpPt_2In_7$, Np_2Ni_{17} and NpBC. For all three compounds we analyze the spin, orbital and total magnetic moments and the total density of states, as well as its projections for selected orbitals and spins. Moreover, for $NpPt_2In_7$ and NpBC we perform the total energy analysis between different magnetic moment arrangements on the Np atoms.