Magnetic properties and electronic structure of $CeRh_{1-x}Pd_xAl$: experiment and calculations

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Our recent studies of CeRhAl suggested an antiferromagnetic ground state below 3.8 K [1]. At low temperatures the magnetic susceptibility χ, and the resistivity ρ indicate an unconventional metallic state in CeRhAl, both quantities exhibit a power law T^{-n} temperature dependencies characteristic of the non-Fermi liquids in the vicinity of the quantum critical point.

CePdAl exhibits an antiferromagnetic phase below T_N = 2.7 K [2] and heavy fermion-like behavior with the specific-heat coefficient $\gamma \equiv C/T = 270$ mJ/molK^2.

The purpose of this work is to discuss $CeRh_{1-x}Pd_xAl$ system of compounds. With the substitution of Rh for Pd we increase by one the number of valence electrons, so we can study the ground state as a function of carrier number. We present the results of the x-ray diffraction analysis and the XPS Ce-*3d* core and valence band spectra. We also present the spin-polarized band structure calculations for CeRhAl, CePdAl and $CeRh_{0.5}Pd_{0.5}Al$ compounds, using the LAPW and LMTO methods. We also present a ground state properties of the system versus x on the phase diagram. The low-temperature properties of $CeRh_{1-x}Pd_xAl$ are discussed on the base of Doradziński-Spałek diagram [3].

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