Electronic structure of CeRhIn₅ and CeIrIn₅

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Recently, a new family of heavy fermion superconductors were discovered, $CeRhIn_5$ [1], $CeIrIn_5$ [2], and $CeCoIn_5$ [3]. $CeRhIn_5$ has an antiferromagnetic ground state which changes to superconducting at a pressure of about 16 kbar. Both $CeIrIn_5$ and $CeCoIn_5$ are ambient-pressure superconductors.

Crystals in this family form as $Ce_nT_mIn_{3n+2m}$, where T=Rh or Ir, n=1 or 2, and m=1, with a tetragonal structure that can be viewed as n-layers of $CeIn_3$ units stacked sequentially along the c-axis with intervening m-layers of TIn_2 . Therefore, first we present our LAPW results obtained for $CeIn_3$. The calculations predict the magnetic ground state in agreement to the experiment data. In common opinion [4] the quasi 2D layers of $CeIn_3$ produce unconventional superconducting and magnetic ground states.

In view of the contrasting behavior (different ground states) of CeRhIn $_5$ and CeIrIn $_5$, we investigated their electronic band structure. The x-ray photoemission spectroscopy (XPS) valence band spectra are related to the LAPW calculations. For comparison, we also investigated the others compounds having the formula Ce $_2$ RhIn $_8$ and Ce $_2$ IrIn $_8$ which are modification of the respective 1:1:5 systems. We have found and discussed an influence of the lattice parameter and the d-f interatomic hybridization effect on the ground state properties in the series of compounds.

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