Electronic structure of the RPdSb (R=Pr, Nd) compounds.

A. Szytuła[a], A. Jezierski[b], D. Fus[a] and B. Penc[a]

[a]Instutute of Physics, Jagiellonian University, Reymonta 4, 30-059 Kraków

[b]Institute of Molecular Physics, Polish Academy of Sciences, 60-179 Poznań

9.7 cm

Electronic structure of the ternary RPdSb (R=Pr, Nd) compounds was studied by the X-ray photoelectron spectroscopy (XPS). Core-levels and valence bands were investigated. The XPS valence bands are compared with the ones calculated using the spin-polarized tight-binding linear muffin-tin orbital (TB LMTO) method. The obtained results show that the valence bands are determined mainly by the Pd 4d band. The calculation of the total energy for two models of the crystal structure: an ordered of the LiGaGe-type and a disordered one of the $CaIn_2$-type indicates that in the RPdSb (R=Pr, Nd) compounds the LiGaGe-type of structure is stable. The spin-orbit splitting values determined from the XPS spectra of Pr and Nd $3d_{5/2}$ and $3d_{3/2}$ are equal to 20.6 eV for PrPdSb and 23.0 eV for NdPdSb. The analysis of these spectra on the basis of the Gunnarsson-Schönhammer model gives information on the hybridization of 4f orbitals with the conduction band, which is large for PrPdSb. Calculated value of the Pr magnetic moment is smaller than that of the free Pr^{3+} ion value, whereas the Nd magnetic moment is equal to the free Nd^{3+} ion value.

13.4 cm

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Corresponding author :
A. Szytuła

Address for correspondence :
Instutute of Physics, Jagiellonian University, Reymonta 4, 30-059 Kraków

Email address :
szytula@if.uj.edu.pl