

Electronic structure and magnetic properties of $\text{Ce}_2\text{Pd}_{1-x}\text{Co}_x\text{Si}_3$ and $\text{Ce}_2\text{Pd}_{1-x}\text{Fe}_x\text{Si}_3$

G. Kozłowski¹ and A. Jezierski²

¹*Faculty of Technical Physics, Poznań University of Technology
Nieszawska 13A, 60-965 Poznań, Poland*

²*Institute of Molecular Physics, Polish Academy of Sciences
M. Smoluchowskiego 17, 60-179 Poznań, Poland*

The electronic structure and magnetic properties of intermetallic phase $\text{Ce}_2\text{Pd}_x\text{Co}_{1-x}\text{Si}_3$ and $\text{Ce}_2\text{Pd}_x\text{Fe}_{1-x}\text{Si}_3$ have been investigated. We used the self consistent tight-binding linear muffin-tin orbital (TB-LMTO) method in the atomic-sphere-approximation (ASA) [1] and the

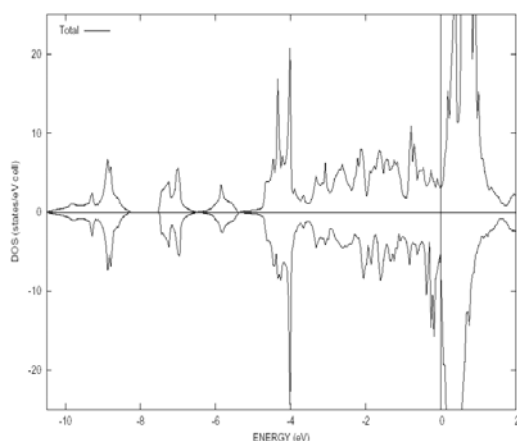


Fig. 1. Total density of states of $\text{Ce}_2\text{Pd}_{0.5}\text{Fe}_{0.5}\text{Si}_3$.

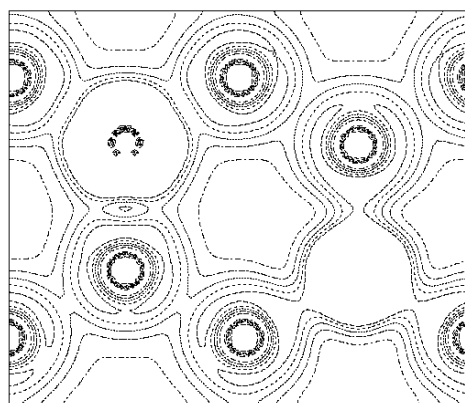


Fig. 2. Charge density of $\text{Ce}_2\text{Pd}_{0.75}\text{Fe}_{0.25}\text{Si}_3$ in plane (002).

Korringa-Kohn-Rostoker (KKR) method with the coherent potential approximation (CPA) [2]. The electronic properties of $\text{Ce}_2\text{Pd}_{1-x}\text{Co}_x\text{Si}_3$ and $\text{Ce}_2\text{Pd}_{1-x}\text{Fe}_x\text{Si}_3$ alloys were calculated for the experimental lattice parameters [3]. Total density of states (Fig. 1), band structure and charge density plots (Fig. 2) were used to describe the fundamental properties of investigated systems.

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Name of the presenting author (poster session II): Grzegorz Kozłowski
e-mail address: mrowek_z@wp.pl
<http://www.put.poznan.pl>