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Electronic structure and Fermi surface of PrMIn$_5$ (M=Co, Rh, and Ir) compounds[1] SAAD ELGAZZAR, Uppsala University, INGO OPAHLE, MANUEL RICHTER, PETER OPPENEER — We report density functional calculations of the electronic structure, Fermi surface, and de Haas-van Alphen (dHvA) quantities of the PrMIn$_5$ (M=Co, Rh, and Ir) compounds. Our investigation is carried out within the framework of the local density approximation (LDA), using a relativistic, full-potential band structure method (FPLO). A critical analysis of the electronic structures and the de Haas-van Alphen quantities is performed, which shows that good agreement with recent measurements is obtained when we assume the Pr $4f$-states to be localized. The topology of the Fermi surface is calculated to be similar to that of non-$4f$ reference compounds, as, e.g., LaRhIn$_5$. The similarities of the Fermi surfaces and the dHvA extremal orbits among the compounds in the series are discussed. We furthermore compare our calculated effective masses with experimental measurements and discuss the differences between them.

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