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Ab initio study of de Haas van Alphen effect in $BaRh_2P_2$ and $BaIr_2P_2$ SIMON BLACKBURN, MICHEL COTE, BOBBY PREVOST, ANDREA BIANCHI, Departement de physique, Universite de Montreal, QC, Canada, MAREK BARTKOWIAK, Paul Scherrer Institut-LDM, PSI, Switzerland, BEATE BERGK, OLEG IGNATCHIK, JOCHEN WOSNITZA, Dresden High Magnetic Field Laboratory, Forschungszentrum Dresden, Rossendorf, Germany, GABRIEL SEYFARTH, Univ Geneva, DPMC, CH-1211 Geneva, Switzerland, CIGDEM CAPAN, ZACHARY FISK, Department of Physics & Astronomy, University of California Irvine, Irvine, CA, USA — The de Haas-van Alphen (dHvA) effect is a powerful probe of the Fermi surface (FS) of a metal. Since it measures the area of a cross-section of the Fermi surface, a theoretical description of this surface complements well these experiments. However, a very accurate description of the FS is required from the ab initio calculations in order to calculate the dHvA frequencies. This is achieved using maximally localized Wannier functions (MLWF) (Marzari & Vanderbilt, *Phys. Rev. B*, 56, 12847)to interpolate the Hamiltonian on a dense k-point grid. In this work, we present a dHvA study of $BaRh_2P_2$ and of its isovalent material $BaIr_2P_2$, both structurally analog to the iron pnictide $BaFe_2As_2$. We also present results concerning $LaFe_2P_2$ and $CeFe_2P_2$ which are also related to $BaFe_2As_2$ by a rigid electronic band shift to account for the difference in the number of electrons.

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