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Ab initio study of de Haas van Alphen effect in LaFe2P2 and CeFe2P2 SIMON BLACKBURN, MICHEL COTE, BOBBY PREVOST, GABRIEL SEYFARTH, ANDREA D. BIANCHI, Universite de Montreal, CIGDEM CAPAN, ZACHARY FISK, University of California Irvine, ROY G. GOODRICH, George Washington University, MAREK BARTKOWIAK, OLEG IGNATCHIK, JOCHEN WOSNITZA, Forschungszentrum Dresden — The use of the maximally localized Wannier functions (MLWF) scheme (Marzari & Vanderbilt, *Phys. Rev. B*, 56, 12847, 1997) to interpolate the Hamiltonian on a very dense k-point grid allows an accurate description of the Fermi surface (FS) of a metal. It is then possible to calculate sections of a FS with great precision. These areas are related to de Haas van Alphen (dHvA) frequencies which can be measured experimentally. In this work, we study LaFe2P2 and CeFe2P2, both crystals in the pnictide family. Results of dHvA frequencies for different functionals are compared directly to experimental data. More specifically, we will present the effects of including a Hubbard U term in the calculations in order to take into account strong correlation on the Fe d orbitals. We will also consider another approach to deal with these orbitals by adding a certain amount of exact exchange to the functional. In this case, we used a PBE0 functional which adds 25% of exact exchange (M. Ernzerhof and G.E. Scuseria, *J. Chem. Phys.*, 110, 5029, 1999).

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