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Electronic and magnetic properties of the uranium and plutonium dipnictides R. C. ALBERS, JIAN-XIN ZHU, S. RUDIN, Los Alamos National Laboratory, M. D. JONES, SUNY at Buffalo, A. K. MCMAHAN, Lawrence Livermore National Laboratory, J. M. WILLS, Los Alamos National Laboratory — First-principles electronic structure calculations have been performed for uranium and plutonium dipnictides based on density functional theory. The magnetism in these compounds is investigated first with spin-polarization only and then also with an orbital-polarization correction. It is found that the inclusion of the orbital-polarization correction improves the comparison between theory and experiment. The Fermi surface topology and the determination of extremal orbitals are also presented.

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