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Effects of correlations in LiFeAs and LiFeP JOHANNES FERBER, KATERYNA FOYEVTSOVA, HARALD O. JESCHKE, ROSER VALENTI, Institut fuer Theoretische Physik, Goethe-Universitaet Frankfurt, 60438 Frankfurt, Germany — We will discuss the role of electronic correlations in the iron-based superconductors LiFeAs and LiFeP by considering the effects on band structure, mass enhancements, and Fermi surface in the framework of density functional theory combined with dynamical mean field theory calculations. We show that LiFeAs shows characteristics of a moderately correlated metal and that the strength of correlations is mainly controlled by the value of the Hund's rule coupling J. The hole pockets of the Fermi surface show a distinctive change in form and size with implications for the nesting properties. We discuss our results in view of recent angle-resolved photoemission spectroscopy and de Haas-van Alphen experiments.

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