

Effects of correlations on the Fermi surface topology of LaFePO, LiFeP and LiFeAs

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We performed charge self-consistent LDA+DMFT (density functional theory combined with dynamical mean field theory) calculations to study correlation effects on the Fermi surfaces of the iron pnictide superconductors LaFePO, LiFeP [1] and LiFeAs [2]. We find a distinctive change in the topology of the Fermi surface in LaFePO and LiFeP where a hole pocket with Fe d_{z^2} orbital character changes its geometry from a closed shape in LDA to an open shape upon inclusion of correlations. In LiFeAs correlations influence mostly the shape of the hole pockets. We discuss our results in the context of angle-resolved photoemission spectroscopy and de Haas van Alphen observations.

[1] J. Ferber, H. O. Jeschke, and R. Valentí, *Fermi surface topology of LaFePO and LiFeP*, Phys. Rev. Lett. **109**, 236403 (2012).

[2] J. Ferber, K. Foyevtsova, R. Valentí, and H. O. Jeschke, *LDA+DMFT study of the effects of correlation in LiFeAs* Phys. Rev. B **85**, 094505 (2012).