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Fermi-Surface Reconstruction in the collapsed-tetragonal phase of KFe2As2 LIMIN WANG, YASUYUKI NAKAJIMA, XIANGFENG WANG, Univ of Maryland-College Park, JASON JEFFRIES, Lawrence Livermore National Laboratory, JOHNPIERRE PAGLIONE, Univ of Maryland-College Park — Recent experiments reveal that applying pressure to KFe2As2 produces a rich phase diagram that includes the reversal in pressure dependence of Tc and without electronic structure change [1] and evolution of structural properties. Inspired by these, we investigate the electronic structure of KFe2As2 as a function of pressure using first-principles theory. Comparing with the ambient pressure tetragonal phase, we find that the Fermi surface topology undergoes significant changes at high pressures, with possible Lifshitz transition in the Fermi surface at high pressure. Together, our results suggest an interesting scenario of superconductivity in this material.

[1] F. Tafti et al., Nat. Phys. 6, 349 (2013).

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