

Abstract Submitted
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Electronic structure and quantum critical behavior of NbFe₂
BRIAN NEAL, WARREN PICKETT, University of California, Davis — The C14 hexagonal Laves phase compound NbFe₂ sits on the edge of a magnetic instability. By varying the composition, Nb_{1-y}Fe_{2+y} encompasses two ferromagnetic states, a spin density wave state, and a quantum critical point ($y = -0.04$). Density functional calculations, using the generalized gradient approximation, found the electronic structure. An analysis of electronic structure calculations will be presented, illuminating the magnetic behavior and susceptibility at low temperature.

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