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Electronic structure and quantum critical behavior of NbFe₂
BRIAN NEAL, ERIK YLVISAKER, 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, an antiferromagnetic or spin density wave state, and a quantum critical point ($y = -0.015$). The electronic structure has been studied using density functional methods. The energy-minimizing structural parameters significantly differ from experimental values. We investigate a flat region in the band structure near the Fermi energy, for possible connection to quantum criticality. Fixed spin moment calculations reveal the character of magnetic moments at the two distinct Fe sites.

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