

Abstract Submitted
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A $1D_s \times 1D_c$ Heisenberg-Kondo Lattice compound $Nb_{12}O_{29}$ ¹ WARREN PICKETT, University of California Davis, KWAN-WOO LEE, Korea University — Local moments embedded in conducting systems form a rich platform for unusual phases, with phenomena including Kondo, heavy fermion, and non-Fermi liquid physics. Using first principles based methods and the refined crystal structure based on columns of 3×4 planar units of NbO_6 octahedra, we determine that mixed valent $Nb_{12}O_{29}$ displays tightly bound local moments forming spin chains along one direction criss-crossed by conducting “nanowires” in the perpendicular direction. Just how local moments – very rare for Nb – emerge and coexist with itinerant electrons, an enigma for decades in this system, is elucidated based on the local structure of the NbO_6 octahedra and orbital+spin ordering. The resulting $1D_s \times 1D_c$ Heisenberg-Kondo lattice (s =spin, c =charge) picture will be discussed.

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Warren Pickett
University of California Davis

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