Lanthanide-like localization of 4d-derived spins in a columnar itinerant niobium oxide lattice

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Local moments embedded in conducting media form a rich platform for unusual phases, with phenomena including Kondo systems, heavy fermion metals and superconductors, and still unexplained non-Fermi liquid behavior. Two decades ago it becameclear that the suboxide $Nb_{12}O_{29}$ displayed local spins in a conducting background, but the origin has remained a conundrum and its low temperature behavior has not beenstudied extensively. Using first principles based methods and the refined crystal structure based on columns of 3×4 planar blocks of NbO_6 octahedra, we find that orthorhombic (o)-$Nb_{12}O_{29}$ introduces a new class of transition metal oxide. The electronic system consists of aNb dimer spin-orbital comparable in size to those in metallo-organic compounds, yet is tightly bound and weakly interacting with itinerant electronic bands. These local moments - a rare occurrence for Nb - form one-dimensional spin chains that criss-cross perpendicularly oriented conducting "nanowires." The local moment bandwidth is comparable to what is seen in rare earth compounds with extremely localized orbitals. The microscopic origin is elucidated based on the local structure of the NbO_6 octahedra and orbital+spin ordering. The resulting anisotropic two-dimensional Heisenberg-Kondo lattice model provides a new and distinctive spin-fermion lattice system for further study.