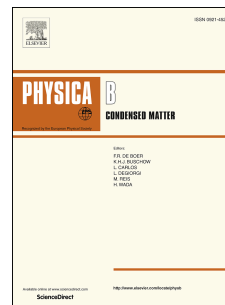


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# Strong spin-orbit effects in transition metal oxides with tetrahedral coordination

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## Abstract

To prove that spin-orbit coupling can play a relevant role in determining the magnetic structure of transition metal oxides with tetrahedral coordination, we investigate the  $d^1$  Mott insulator  $\text{KOsO}_4$ , combining density functional theory calculations and the exact diagonalization approach. We find that the interplay between crystal field, strong spin-orbit coupling, electronic correlations and structural distortions brings the system towards an antiferromagnetic phase, characterized by a non-vanishing orbital angular momentum and anisotropy among the in-plane and the out-of-plane antiferromagnetic correlations. We also show that, due to the peculiar interplay between spin-orbit coupling, Hund’s coupling and hopping connectivity the system is on the verge of developing short range ferromagnetic correlations marked by strong directionality.

*Keywords:* Spin orbit coupling, electron-electron correlations, transition metal oxides

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