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

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We analyze the effects of strong spin-orbit coupling (SOC) in heavy transition metal oxides with tetrahedral coordination and eg^1 configuration. We show that the interplay between strong Hubbard interaction, large SOC strength and crystal field leads to an unquenched orbital momentum and a deviation from a conventional s=1/2 Heisenberg antiferromagnet, to an extent that crucially depends on the ratio between the microscopic parameters. The specific case of the insulating $KOsO_4$ is analyzed by combined ab-initio and exact diagonalization approaches. We show that, due to the peculiar hopping connectivity and structural deformation, an entangled spin/orbital state emerges, which is marked by strong anisotropy.

References:

[1] D. Pesin and L. Balents, Nat. Phys. **6**, 376 (2010)