Magnetic structure and superexchange pathways in CsV_2O_5

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The study of low dimensional spin-1/2 quantum systems has been a very prolific field of condensed matter physics during the last decades. The family of vanadates, in particular, has provided a rich variety of compounds with different behaviours and topologies.

Their magnetic structure and properties are primarily determined by the magnitude and the sign of the different exchange couplings arising between magnetic ions and therefore on the very details of their atomic and electronic structures. The sole consideration of the topology of a compound, based on idealized crystal structures, is often incomplete and even misleading.

In this work, the magnetic properties of the layered compound CsV_2O_5 have been investigated using density-functional calculations. The results show that this compound is built from strongly dimerized alternating chains oriented along the **c** axis. Moreover, we demonstrate that the largest interaction along the chains direction arises *between* the structural dimers, involving a superexchange pathway through the covalently bonded $V^{(5+)}O_4$ bridging groups. These results should motivate further experimental investigations of the magnetic excitations in this compound.