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Theoretical study of the electronic and magnetic properties of β-$TeVO_4$ ANDRES SAUL, CINaM/CNRS Université dÁix Marseille and CEE MIT, GUILLAUME RADTKE, IMPMC/CNRS Université Pierre et Marie Curie — The β phase of this compound can be described by zigzag chains formed by VO_5 distorted square pyramids sharing corners. This oxide, with V^{4+} ions as magnetic centers, can be thus seen as a realization of a quasi-one-dimensional Heisenberg S=1/2 Hamiltonian. The corner-sharing of the VO_5 pyramids could lead to the prediction of AFM nearest neighbor interactions mediated by a weak super-exchange mechanism opening the possibility of complex magnetic properties due to competing next nearest-neighbors or inter-chain interactions. In this work we have studied its electronic and magnetic properties using density functional calculations. In particular, we evaluated the magnetic couplings on the basis of broken-symmetry formalism. We have performed extensive calculations comparing the results of the standard GGA (PBE) functional to the hybrid PBE0 functional and two different GGA+U implementations (SIC and AMF). The overall picture that arises from our calculations is of a frustrated AFM system with small FM nearest neigbors interactions but larger AFM nearest neighbors couplings. We discuss our results in the framework of the Kugel-Khomskii model using a projection of the electronic structure in localized Wannier functions.

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