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Benchmark study of the application of density functional theory to correlated t_{2g}^1 vanadates DANILO PUGGIONI, JAMES RONDINELLI, Drexel University — $SrVO_3$ and $CaVO_3$ are strongly correlated perovskite-structured metals belonging to the class of transition-metal oxides with a $3d^1$ electronic configuration. Both cubic $SrVO_3$ and orthorhombically distorted $CaVO_3$ are classified as Pauli paramagnets, yet their magnetic states at low temperature remain controversial. Here, we present and discuss the results of systematic density functional theory (DFT) calculations on the atomic and magnetic structures of both $SrVO_3$ and $CaVO_3$ to shed light on this issue. We use standard and "beyond-DFT" exchange-correlation functionals to evaluate the stable magnetic states. We conclude by discussing both the accuracy of these methods for reproducing the atomic structures of the t_{2g}^1 vanadates and their implications on artificially structured oxide superlattices.

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