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Electronic correlations in monolayer VS_2 ERIC B. ISAACS, CHRIS A. MARIANETTI, Department of Applied Physics and Applied Mathematics, Columbia University — The layered transition metal dichalcogenide vanadium disulfide (VS_2), which nominally has 1 electron in the $3d$ shell, is potent for strong correlation physics and is possibly another realization of the one-band Hubbard model beyond the cuprates. Here we investigate the octahedral (OCT) and trigonal prismatic (TP) phases of monolayer VS_2 using density functional theory plus Hubbard U calculations. Unlike the OCT phase, the TP phase has an isolated low-energy band due to the crystal field splitting and the nearest-neighbor V-V hopping. Within DFT, ferromagnetism spin splits this band leading to a low-band-gap $S = 1/2$ ferromagnetic insulating TP phase, which is lower in energy than the OCT phase. The on-site interaction U, which we find to be approximately 4 eV via linear response, increases the band gap, leads to Mott insulating behavior, and for sufficiently high values stabilizes the ferromagnetic OCT phase. We explore the impact of charge density waves in monolayer VS_2 and discuss the possibility to experimentally realize the TP phase.

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