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Orbitally driven trimerization in LiVO_2 and LiVS_2 : a “partial Mott transition” HUA WU, D.I. KHOMSKII, University of Cologne, Germany — Layered triangular-lattice transition-metal compounds often display interesting magnetic and electronic properties. Here we studied the formation of the trimerized spin-singlet state of the V^{3+} ($S=1$) in vanadates LiVO_2 and LiVS_2 and their electronic structure with a special orbital order, using constrained LSDA+ U calculations combined with lattice optimization. The obtained results show that the trimerization distortion in LiVO_2 increases as the effective U decreases, and the calculated distortion of $\sim 0.3 \text{ \AA}$ at the small $U=1 \text{ eV}$ agrees well with the experiments, indicating that LiVO_2 is close to a metal-insulator transition. The corresponding distortion in LiVS_2 is even stronger, being $\sim 0.4 \text{ \AA}$ at the $U=1 \text{ eV}$, which is due to enhanced electron delocalization via increased V-S covalency, in spite of a lattice expansion. This agrees with the experimental finding that LiVS_2 has a metal-insulator transition. The calculated energy gain associated with the trimerization well accounts for the observed structural phase transition temperature in LiVO_2 and LiVS_2 . We conclude that the trimerization in LiVO_2 and LiVS_2 is due to a partial delocalization of the orbitally ordered electrons—a “partial Mott transition,” occurring not in the whole system but in small clusters (here in trimers). This situation is contrasted with that in NaVO_2 , which is further away from the localized-itinerant crossover and thus remains insulating with different orbital ordering.

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