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Cluster dynamical mean-field theory study on deficient spinel chalcogenide GaV_4S_8 HEUNG SIK KIM, KRISTJAN HAULE, DAVID VANDERBILT, Rutgers Univ — Here I will present my current research progress about a deficient spinel compound GaV_4S_8 (GVS) using a cluster dynamical mean-field (DMFT) approach. GVS has been of growing interest recently because of its multiferroicity below T_C˜13K. It has an additional structural transition around T_f ˜70K, lowering the symmetry of the high-temperature cubic phase to a rhombohedral structure as it is cooled. Across the two structural transitions GVS remains insulating with the gap size estimated to be ˜0.3 eV, and the insulating nature of its high-temperature cubic paramagnetic phase is suspected to be a Mott-type. However, there has not been a systematic study about the Mott-insulating phases of GVS, which should be important to understand the low- temperature ferroelectric and multiferroic phases. Hence we apply a cluster DMFT method to GVS with V_4 as our cluster problem, employing a molecular orbital basis set instead of an atomic one. Comparing with single-V-site DMFT calculations, we show that intra-cluster correlations are essential in reproducing the Mott-insulating phase of the high-T cubic paramagnetic phase. Correlation effects on the crystal structure of GVS will be also discussed, and especially the role of Hund's coupling in tuning V_4-clustering by switching low to high spin states will be shown.

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