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Poster presentation title: A molecular orbital DMFT approach for the insulating nature of a deficient spinel compound GaV4S8

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Abstract: In this study, we investigate paramagnetic and insulating states of a deficient spinel compound GaV4S8 (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 estimated to be ~0.3 eV, and the insulating nature of its high-temperature cubic 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 V4 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, and further demonstrate the role of Hund's coupling in reducing the gap size. Correlation effects on the crystal structure of GVS will be also discussed.