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**Antiferromagnetic Exchange, Hunds Coupling and the Origin of the Charge Gap in LaMnPO**[1] DANIEL MCNALLY, J.W. SIMONSON, G.J. SMITH, V. LEYVA, C. MARQUES, M.C. ARONSON, Stony Brook University, K.W. POST, D.N. BASOV, University of California, San Diego, Z.P. YIN, M. PEZZOLI, G. KOTLIAR, Rutgers University, Y. ZHAO, J.W. LYNN, National Institute of Standards and Technology, L. DEBEER-SCHMIDT, A.I. KOLESNIKOV, Oak Ridge National Laboratory — LaMnPO is an antiferromagnetic insulator with an ordering temperature $T_N = 375$ K, ordered moment of 3.2 $\mu_B$/Mn and a charge gap $\Delta = 1$ eV. We present inelastic neutron scattering and magnetization data that are well described by a Heisenberg model of magnetic interactions with nearest neighbour exchange $SJ_1 \sim 39$ meV and next-nearest exchange $SJ_2 \sim 12$ meV. These measurements also show magnetic correlations persist up to $T_{max} \sim 700$ K, significantly larger than $T_N$ due to the effectively decoupled MnP layers. High temperature optical transmission measurements show the charge gap has decreased by $\approx$ 10% by $T_{max}$ suggesting the rather small exchange interactions $J \ll \Delta$ have only a small effect on the gap. Density functional theory and dynamical mean field theory DFT+DMFT reproduce the observed gap in the paramagnetic state of LaMnPO only in the presence of strong Hunds coupling $J_H$, as well as onsite Coulomb interactions U. In light of these experimental and theoretical results, LaMnPO should be considered a Mott-Hunds insulator.

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