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Electron-hole excitations in $CaMnO_3$ and $LaMnO_3$(*) OSCAR D. RESTREPO, ADOLFO G. EGUILUZ, University of Tennessee and ORNL — The electron-hole excitations in $CaMnO_3$ and $LaMnO_3$ are investigated via ab initio techniques (time-dependent density-functional theory). The ground state is described within the LDA+U correlated-band structure method. The electron dynamics is handled within the random-phase approximation (RPA). The loss spectrum in both materials is dominated by a striking collective excitation; the same is directly related to the underlying electronic structure, as its energy is a signature of the relative location of the upper and lower Hubbard bands. The physics of the dynamical screening (the spectral weight of the leading excitation, its remarkable dependence on wave vector (both on the magnitude and direction of q, etc.) is controlled by d-d transitions and the microscopic crystal local fields. Our predictions can be readily verified via measurements of the dynamical structure factor with inelastic scattering of hard x-rays –providing a direct test of the quality of the LDA+U ground state and the RPA dynamics. In fact, there is qualitative agreement with a recent investigation for $LaMnO_3$ with resonant x-ray scattering (**). (*) Research supported by NSF Grant ITR-DMR 0219332 (**) S.Grenier et al., cond-mat/0407326.

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