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Electronic and crystal-field effects in the fine structure of electron energy-loss spectra of $\mathbf{La_xCa_{1-x}MnO_3}$ WEIDONG LUO, MARIA VARELA, JING TAO, STEPHEN J. PENNYCOOK, SOKRATES T. PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory — The fine structure of oxygen K-edge electron energy-loss spectra (EELS) of transition-metal oxides is known to correlate with nominal oxidation states (NOS) that are often interpreted as charge states. We report the results of a systematic study of O K-edge EELS fine structures in $La_xCa_{1-x}MnO_3$ and their evolution as functions of doping x. The calculated spectra, specifically the pre-peak intensities and peak separations, as functions of x are in excellent agreement with experimental data. The calculations show that the variation of the pre-peak's intensity with doping is controlled by the orbital occupancy of the majority-spin Mn $3d$ states while its width is controlled by crystal-field splitting. The energy separation between the pre-peak and the main peak also has a correlation with the doping parameter x and the NOS. The results confirm that the NOS extracted from EELS correlates with orbital occupancies but does not probe physical charges of the Mn sites. This research was sponsored in part by the DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering and by the McMinn Endowment at Vanderbilt University. Computations were performed at the National Energy Research Scientific Computing Center.

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