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Charge-fluctuation excitations in $Na_{1/3}CoO_2 \cdot yH_2O$(*) O.D. RESTREPO(1), A.G. EGUILUZ(1), University of Tennessee and CMSD,ORNL (2), K.-W. LEE, J. KUNES, W.E. PICKETT(3), University of California, Davis — We report a theoretical study of the electron-hole excitation spectrum of the hydrated superconductor $Na_{1/3}CoO_2 \cdot yH_2O$. We use a paramagnetic LDA ground state as our starting point, and calculate the dynamical density-response function using time-dependent density-functional theory. Our results are compared with calculations for the parent compound $Na_{1/3}CoO_2$ and with recent electron-energy loss spectroscopy (EELS) experiments reported by H. X. Yang et al. (PRB 72, 075106 (2005)). Interestingly, the dielectric function obtained from our ab-initio calculations differ appreciably, in the key spectral region, from the one extracted from the experimental loss function by H. X. Yang et al. In fact, our dielectric function shows better qualitative correspondence with the loss data; this finding highlights the relevance of ab-initio calculations for the study of the experimental manifestation of the electronic structure. The physics of the prominent peaks in the loss spectra is discussed; we identify signatures of the underlying electronic structure in the hydrated compounds. (*) DOE-CMSN PCSCS collaboration. (1) Supported by NSF ITR-DMR 0219332 (2) Managed by UT-Battelle for the U.S. DOE under contract DE- AC05-00OR22725. (3) Supported by DOE Grant DE-FG03-01ER45876

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