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Renormalization of f-levels away from the Fermi energy in electron excitation spectroscopies: Density functional results of $\mathbf{Nd_{2-x}Ce_xCuO_4}$ B. BARBIELLINI, Northeastern U., T. JARLBORG, DPMC, University of Geneva (Switzerland), H. LIN, R.S. MARKIEWICZ, A. BANSIL, Northeastern U. — Relaxation energies for photemission, when an occupied electronic state is excited, and for inverse photoemission, when an empty state is filled, are calculated within the density functional theory with application to $Nd_{2-x}Ce_xCuO_4$ (NCCO). The associated relaxation energies are obtained by computing differences in total energies between the ground state and an excited state in which one hole or electron is added into the system. The relaxation energies of f-electrons are found to be of the order of several eV's, indicating that f-bands will appear substantially away from the Fermi energy (E_F) in their spectroscopic images, even if these bands lie close to the E_F in the ground state of NCCO. Our analysis explains why it would be difficult to observe f electrons at the E_F even in the absence of strong electronic correlations. Work supported by the US DOE.

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