

Abstract Submitted
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Effect of local correlation on electron phonon coupling in La_2CuO_4 using LDA+DMFT JULIEN GROULX, PAUL BOULANGER, MICHEL CÔTÉ, Univ of Montreal — ARPES measurements show a kink in the electron dispersion of La_2CuO_4 around 80 meV. The cause of this kink is still under debate. The phonon spectrum is consistent with a kink at that energy but previous studies have demonstrated that the response of the electron-phonon coupling calculated in the framework of density functional theory (DFT) with a GGA functional is too weak to account for the observed kink. However, other works have shown that the electron-phonon coupling can be underestimated by the treatment of LDA/GGA functionals. For this reason, we investigate the effect of the strong local correlation caused by the "d" electrons of Cu on the calculation of electron-phonon matrix elements. The local correlation is added using the dynamic mean-field theory (DMFT) approach within a DFT method. Specific electron-phonon matrix elements are calculated using the Frozen Phonon method.

Julien Groulx
Univ of Montreal

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