

Abstract Submitted
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Assessment of the importance of correlation effects in Li_xNbO_2

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J. KUNES, Univ. of Augsburg — About 15 years ago Geselbract et al. reported
superconductivity with $T_c=5\text{K}$ for $x \approx 0.5$ in Li_xNbO_2 . The critical temperature
does not show significant change in the range $0.45 < x < 0.8$. The electronic
structure is based on a strongly two-dimensional triangular Nb lattice, and the
superconducting phase is hole-doped from $x=1$ band insulator. The strong trigonal
crystal field results in a single Nb d_{z^2} band isolated within a wide gap, giving a
single-band triangular lattice system. The single band has a band width $W=1.7$
eV and hopping parameters $t_1=64, t_2=100, t_3=33$ (in units of meV), showing second
nearest neighbor hopping to be dominant. To study possible correlation effects, we
apply DMFT using on-site Coulomb repulsion $U=0-4$ eV and obtain the spectrum
with MaxEnt. Even $U=1$ eV is found to cause substantial change in the spectrum,
suggesting the importance of correlation effects in Li_xNbO_2 .

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