

Abstract Submitted
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ARPES and NMTO of $\text{Li}_{0.9}\text{Mo}_6\text{O}_{17}$: Implications for Unusually Robust Quasi-One Dimensional Behavior¹ J.W. ALLEN, U. Michigan, L.M. DUDY, Uni Wuerzburg, J.D. DENLINGER, Lawrence Berkeley Nat'l Lab, J. HE, Clemson U., M. GREENBLATT, Rutgers U., M.W. HAVERKORT, MPI Chem. Phys. Dresden, O.K. ANDERSEN, Y. NOHARA, MPI Stuttgart — $\text{Li}_{0.9}\text{Mo}_6\text{O}_{17}$ displays theoretically interesting [1] metallic quasi-one dimensional (1D) behavior that is unusually robust [2] against 3D crossover before superconductivity at $\approx 1.9\text{K}$, and has large anomalous Luttinger liquid density-of states exponent $\alpha \approx 0.6$. We present very high resolution, low temperature ($T \approx 6\text{K}-26\text{K}$) angle resolved photoemission spectroscopy (ARPES) data analyzed with non-linear muffin tin orbital (NMTO) Wannier function band theory. We confirm a previous conclusion [3] that the LDA agrees unusually well with ARPES, implying small Hubbard U , and find in ARPES the dispersion and Fermi surface warping and splitting expected for predicted small but long range inter-chain hoppings ($t_{\perp} \approx 10-15 \text{ meV}$). These various findings imply the likely importance of long range Coulomb interactions for the large α value [4] and reaffirm the great puzzle [2] of quasi-1D behavior well below the 3D crossover T implied by t_{\perp} .

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