

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Sorting Category: 05.4 (C)

DFT Study of the Single-Band Layered TMO LiNbO₂

ERIK YLVISAKER, UC Davis, WARREN PICKETT, UC Davis —
We establish using first principles methods that LiNbO₂ is a realization of a triangular lattice “single band” system. The bandwidth (less than 2 eV) suggests the interesting possibility of correlation effects that should be kept in mind. We present a tight-binding model for the valence band of LiNbO₂, composed primarily of Nb d_{z²} states, finding that intralayer second neighbor hopping t_2 100 meV is dominant over the significantly smaller first neighbor interactions t_1 70 meV. The nearest neighbor coupling is strongly modified by oxygen displacements, and the electron-phonon coupling may provide the coupling mechanism for superconductivity in Li-deficient samples ($T_c \approx 5$ K). We will present the Nb-centered Wannier function, which provides insight into this unusual electronic structure. Calculations of the Born effective charges for the metal ions are also found to have anisotropy that reflects the layered nature of the electronic bonding. Their deviation from formal charge values indicates important covalent character, which is also evident in the Wannier function.

Prefer Oral Session
 Prefer Poster Session

Erik Ylvisaker
eylvisaker@physics.ucdavis.edu
UC Davis

Date submitted: 30 Nov 2005

Electronic form version 1.4