Assessment of Correlation Effects in $\text{Li}_x\text{NbO}_2$

Kwan-woo Lee (UC Davis)
Jan Kunes (Augsburg)
Richard T. Scalettar (UC Davis)
Warren E. Pickett (UC Davis)

• transition metal oxide
• layered structure
• triangular lattice
• superconductor

Acknowledgement
Erik R. Ylvisaker, Simone Chiesa
Outline

Introduction
1. Crystal Structure
2. Observations
3. Electronic Structure
4. Calculation

Results
1. Occupancy vs. chemical potential
2. U-dependent spectral density
3. Effect of O displacement on spectral density

Conclusion
Structure of LiNbO$_2$

- Double-layered hexagonal structure
- Quasi-2D structure: $c/2=1.8a$
- Nb triangular lattice
- Trigonal prismatic coordination of NbO$_6$

G.T. Liu et al., PRB 74, 012504 (2006).
There are no systematic doping studies yet.
Superconducting Li$_x$NbO$_2$: $0.45 \leq x < 0.80$

- At $x=0.68$, specific heat measurements show BCS s-wave superconductivity

- At $x=0.5$, Deformation Potential (Raman active mode):
  - near $\Gamma$ 8 eV/$\text{Å}$
  - near $K$ 1.6 eV/$\text{Å}$

$\gamma = \frac{\gamma_{\text{exp}}}{\gamma_{\text{band}}} - 1 \approx 0.48$

⇒ phonon-mediated pairing
**LiNbO$_2$ Electronic Structure**


2D Tight-Binding

Tight binding fit shown dashed

### Single Nb d($z^2$) band

- Lower half of weight is localized within 0.2 eV width.

### TB parameters (meV)

<table>
<thead>
<tr>
<th></th>
<th>$t_1$</th>
<th>$t_2$</th>
<th>$t_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>64</td>
<td>100</td>
<td>33</td>
</tr>
</tbody>
</table>

$\Gamma - M - K$
Question & Calculation

- Is NbO$_2$ (no lithium) a Mott-insulator?
- How much does the spectral density change due to correlation effects?
  
  \[
  \begin{aligned}
  n=1 & \quad (\text{NbO}_2) \\
  n=4/3 & \quad (\text{Li}_{1/3}\text{NbO}_2) \\
  n=5/3 & \quad (\text{Li}_{2/3}\text{NbO}_2)
  \end{aligned}
  \]

- Single-band simulation including three hopping parameters; $t_1=64$, $t_2=100$, $t_3=33$ (in meV)
  \[ W \approx 1.5 \text{ eV} \]

- QMC-DMFT
  \[ T=1100 \text{ K (0.1 eV)} \]

- MaxEnt $\Rightarrow$ Spectral density
Already at $U=1$ eV, a saddle point appears near half-filling.

At $U=1.5$ eV, the saddle point becomes a plateau.

Also, compressibility nearly vanishes at $U=1.5$ eV, indicating onset of insulating state.
U-dependent Spectral Density at $n=1$

- At $U=1.5$ eV, a gap opens clearly. $\Rightarrow U_c \approx 1.4$ eV
- A hump develops simultaneously with MIT just below the Fermi energy.
Correlated behavior appears already at $U=0.5$ eV.

A robust LHB and a structure at $E_F$ appear simultaneously at $U=1$ eV.

For $n$ nearer half-filling, there is more weight in the LHB.

Consistent with the existing X-ray spectra by Cherkashenoko et al. (Z. Phys. B 93, 417 (1994)), but more PES is needed.
Effect of O Displacement on Spectral Density

At $n=5/3$, stronger variation near $E_F$.
At $n=4/3$, some structure occurs just above $E_F$.
No clear evidence of importance for superconductivity.
Summary

- The single-band, triangular lattice system $\text{Li}_x\text{NbO}_2$ has been studied with LDA+DMFT method.
- At half-filling, MIT occurs at $U_c \approx 1.4$ eV.
- Even at $U=1$ eV, the spectral density changes significantly reflecting clear correlation effects.

Photoemission data are needed, at various temperatures to compare and determine how important the correlation effects are.