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Assessment of Correlation Effects in Li_xNbO_2

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

Acknowledgement

Erik R. Ylvisaker, Simone Chiesa

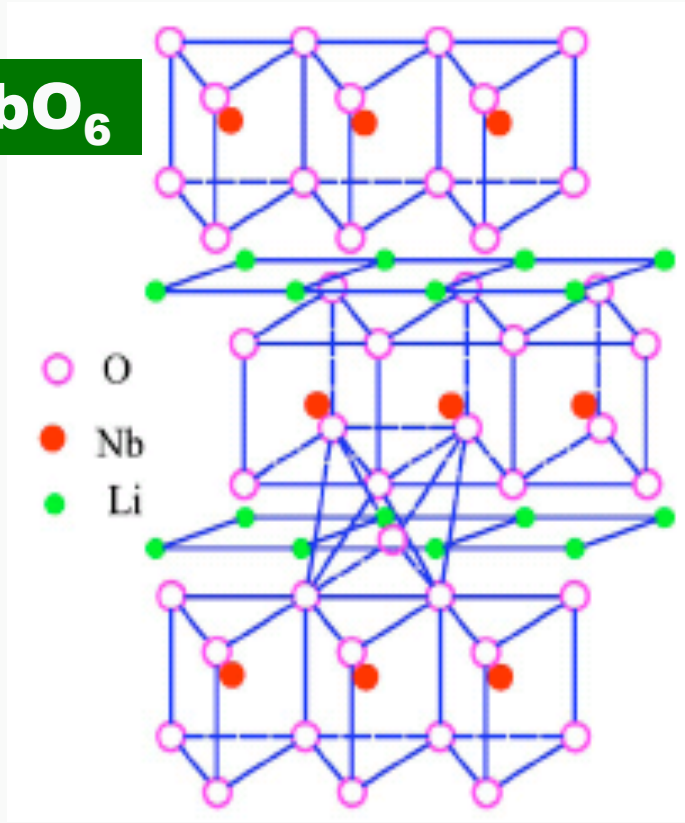
Outline

- **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**

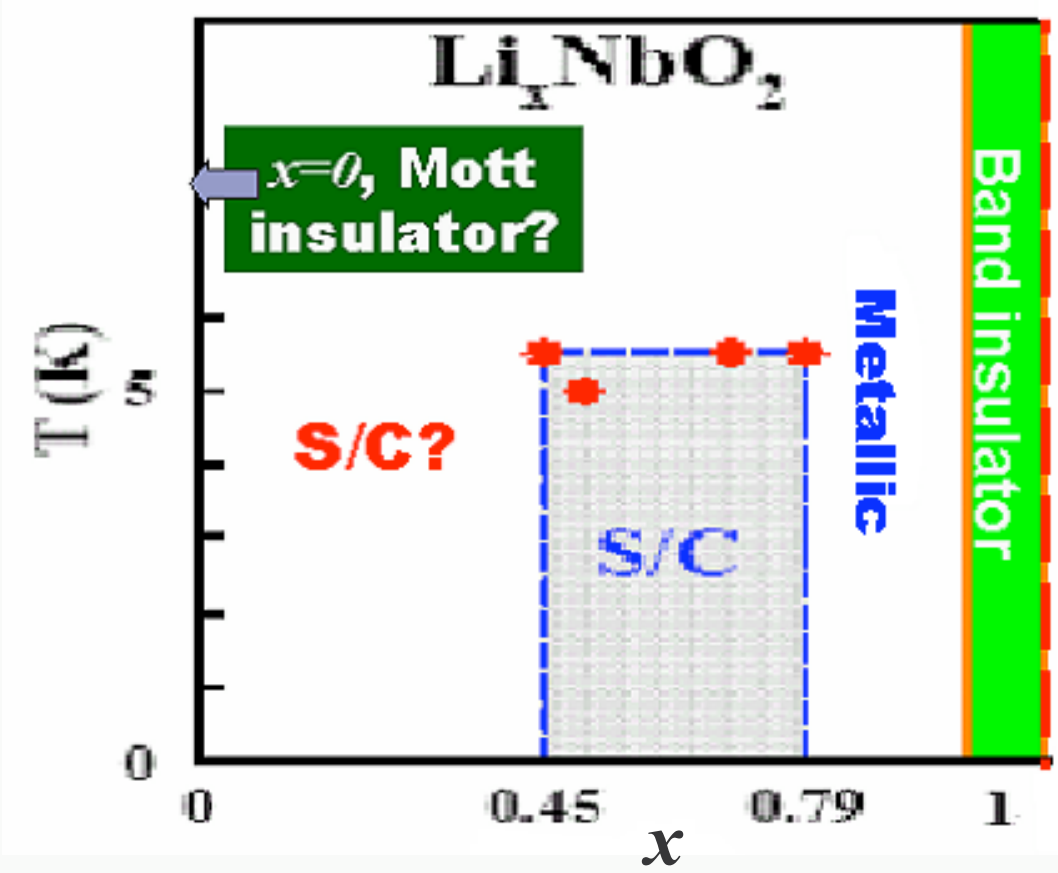
Structure of $LiNbO_2$



G.T. Liu et al., PRB 74, 012504 (2006).

- Double-layered hexagonal structure
- Quasi-2D structure: c/2=1.8a
- Nb triangular lattice
- Trigonal prismatic coordination of NbO_6

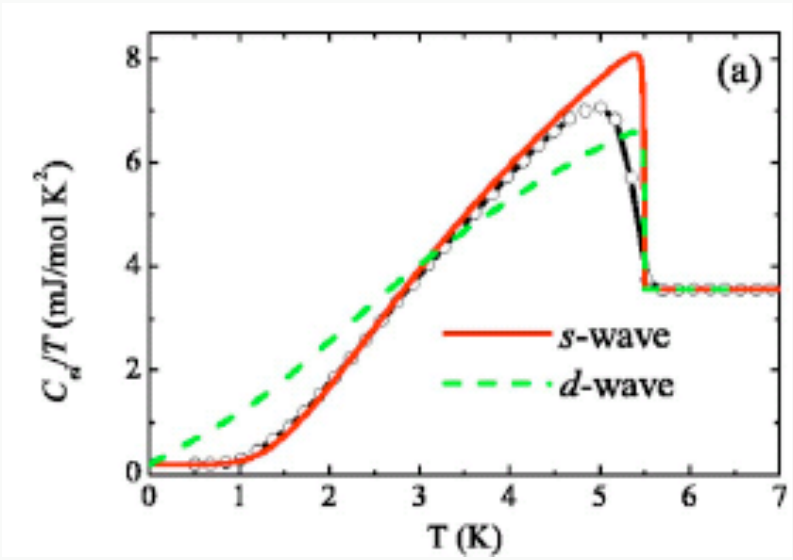
Phase diagram



Geselbracht et al., Nature 345, 324 (1990); Moshopoulou et al., PRB 59, 9590 (1990); Liu et al., PRB 74, 012504 (2006).

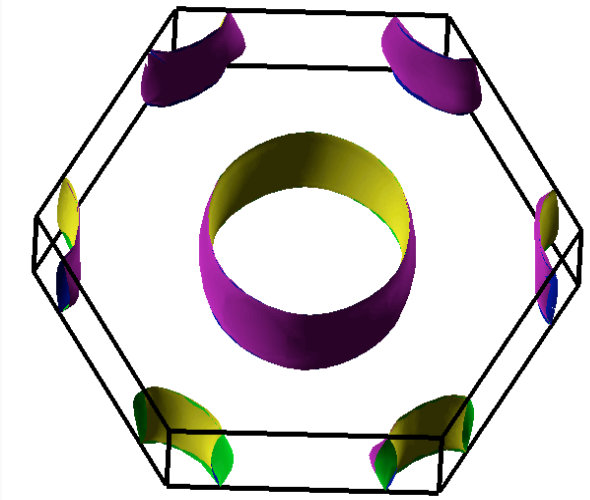
- **There are no systematic doping studies yet.**

Superconducting Li_xNbO_2: $0.45 \leq x < 0.80$



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

G.T. Liu et al, PRB 74, 012504 (2006).



- At $x=0.5$, Deformation Potential (Raman active mode):
  near Γ 8 eV/Å
  near K 1.6 eV/Å

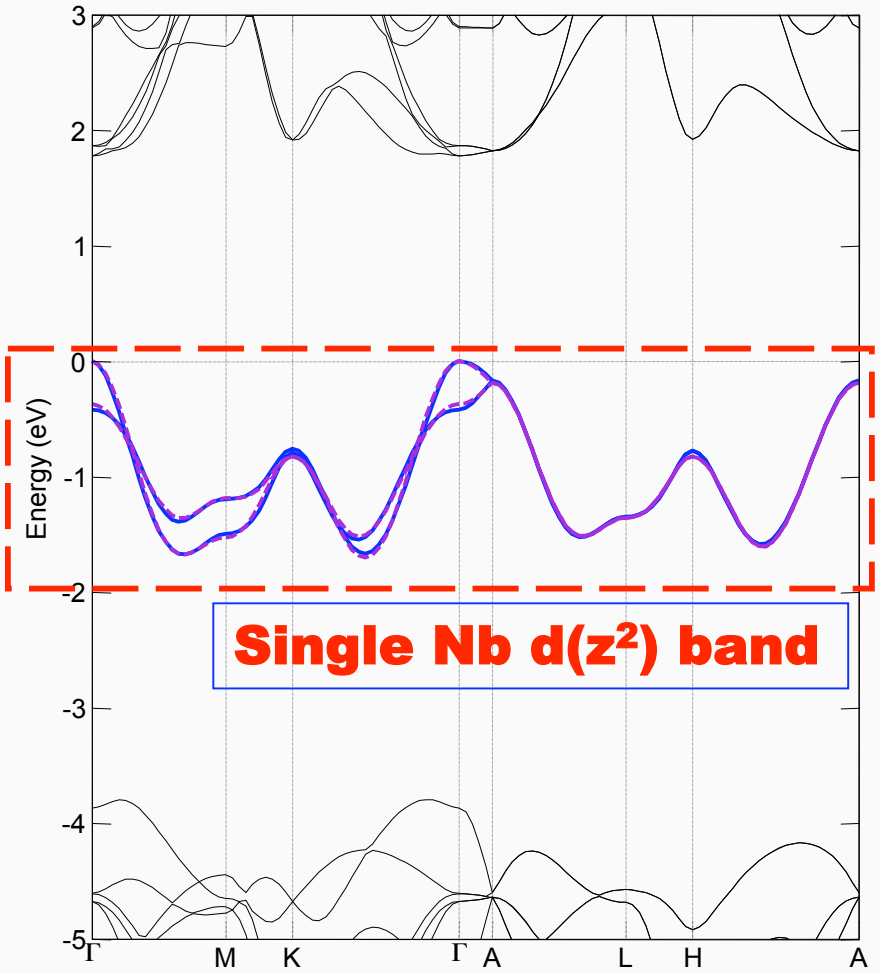
E.R. Ylvisaker and W. E. Pickett, (unpublished)

- At $x=0.68$, $\lambda=\gamma_{exp}/\gamma_{band}-1\approx0.48$

⇒ phonon-mediated pairing

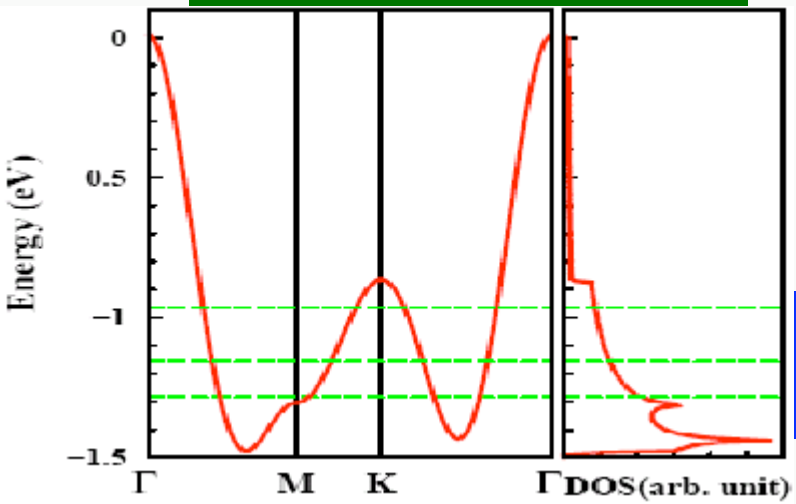
$LiNbO_2$ Electronic Structure

E.R. Ylvisaker and W.E. Pickett, PRB 74, 075104 (2006).



Tight binding fit shown dashed

2D Tight-Binding



x=2/3
x=1/3
x=0

TB parameters (meV)		
t_1	t_2	t_3
64	100	33

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

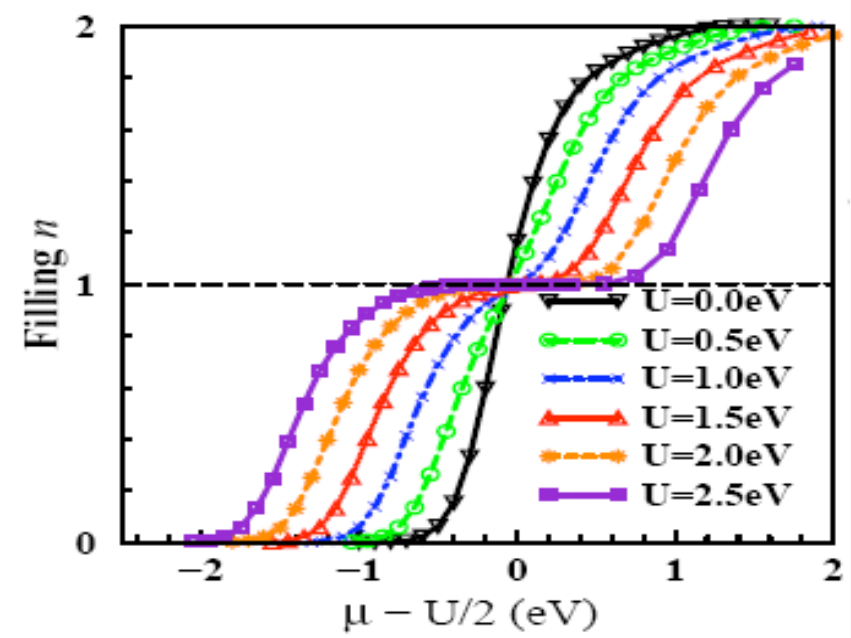
Question & Calculation

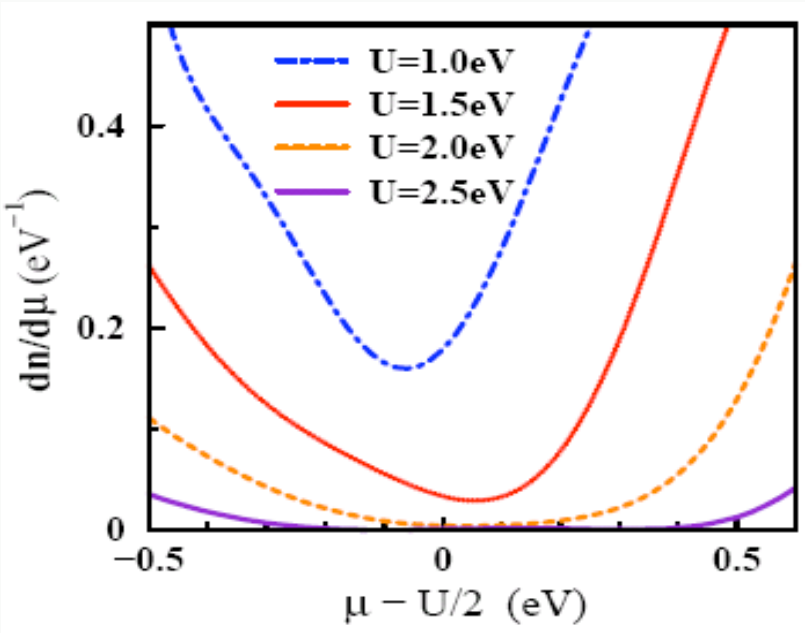
- Is NbO_2 (no lithium) a Mott-insulator?
- How much does the spectral density change due to correlation effects?
- n=1 (NbO_2)
  n=4/3 ($Li_{1/3}NbO_2$)
  n=5/3 ($Li_{2/3}NbO_2$)

- Single-band simulation including three hopping parameters; t_1=64, t_2=100, t_3=33 (in meV)
  ⇒ W ≈1.5 eV
- QMC-DMFT
  T=1100 K (0.1 eV)
- MaxEnt ⇒Spectral density

M. Jarrell and J. E. Gubernatis, Phys. Rep. 269, 133 (1996).

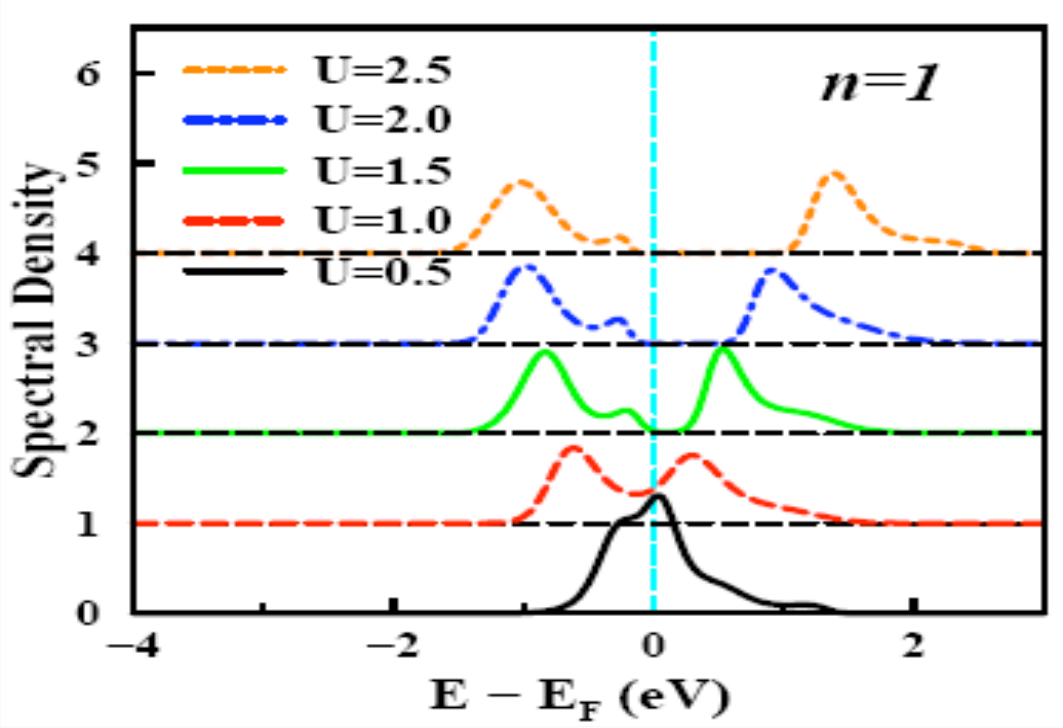
Electron Filling & Compressibility vs. μ





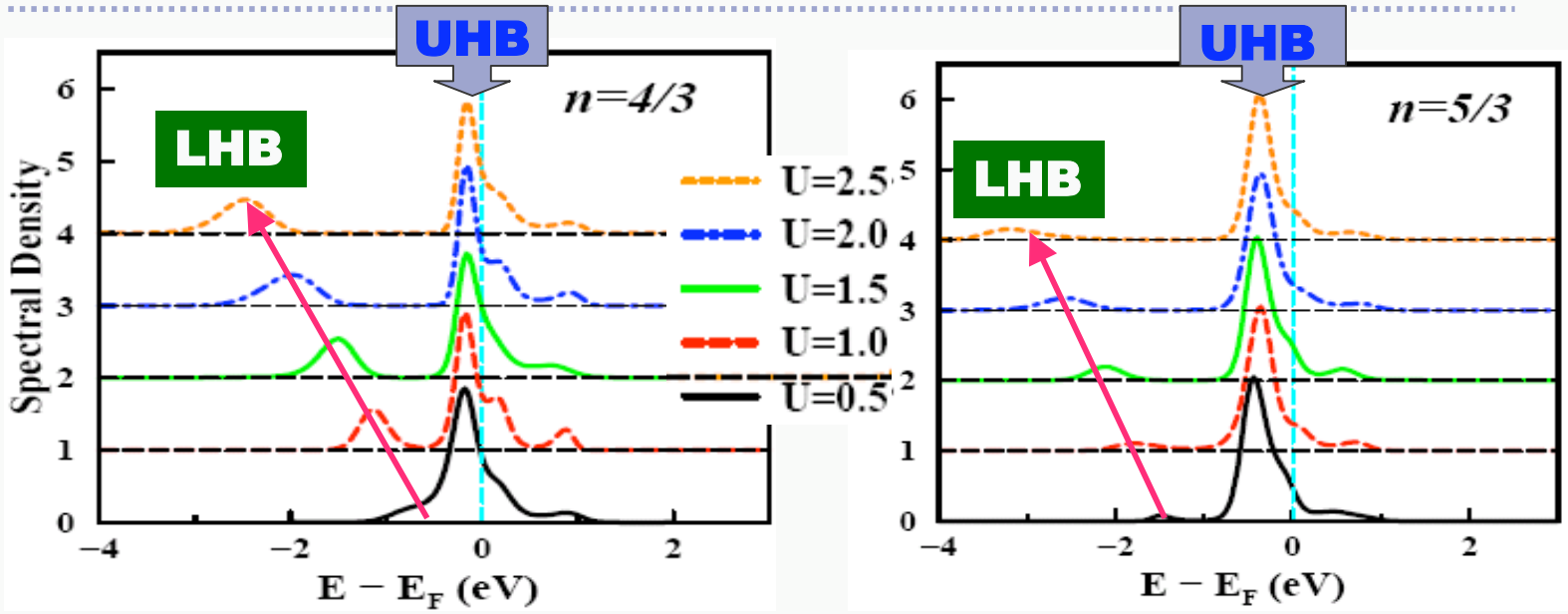
- Already at U=1 eV, a saddle point appears near half-filling.
- At U=1.5 eV, the saddle point becomes a plateau.
- Also, compressibility nearly vanishes at U=1.5 eV, indicating onset of insulating state.

U-dependent Spectral Density at *n=1*



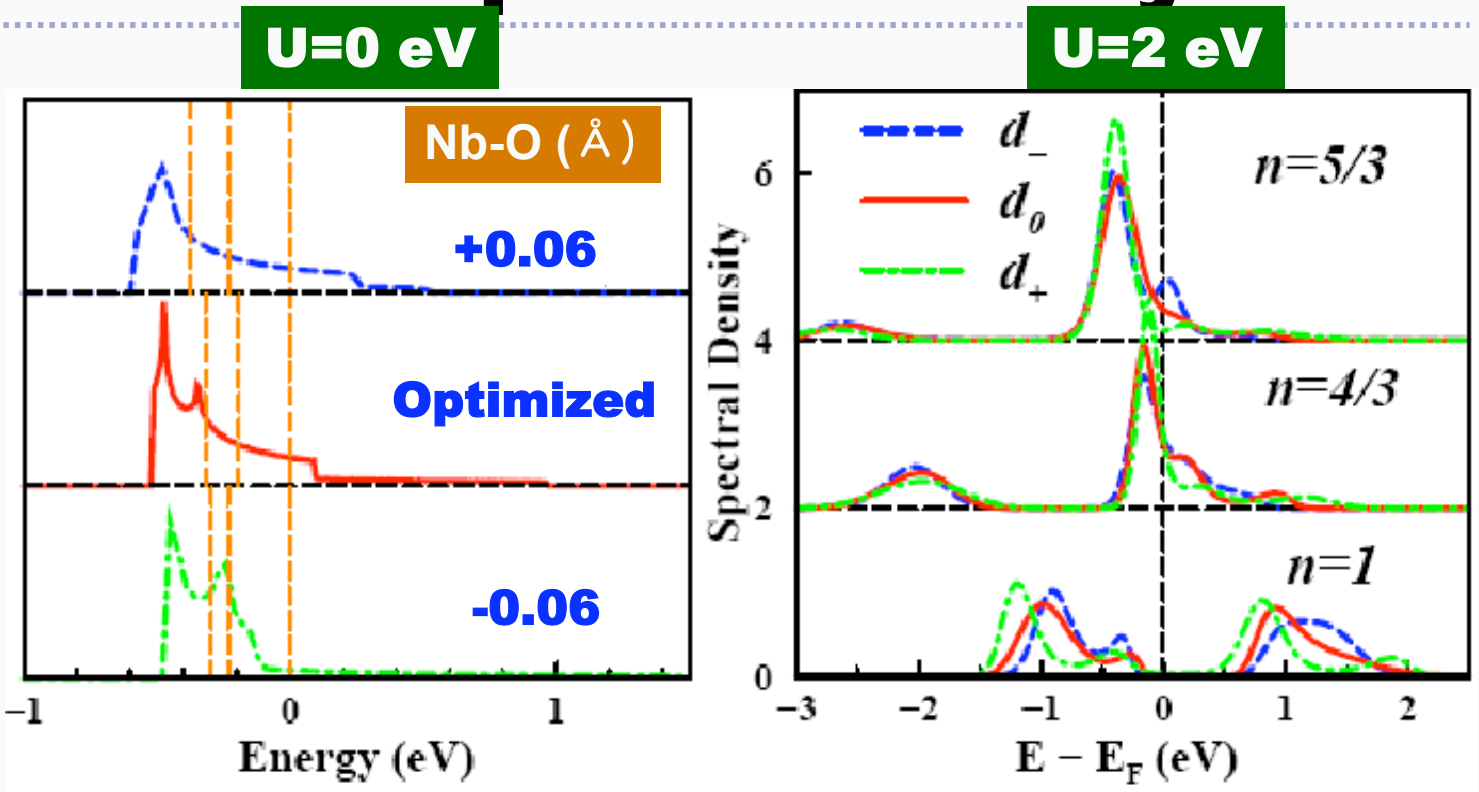
- At U=1.5 eV, a gap opens clearly. ⇒ $U_c \approx 1.4$ eV
- A hump develops simultaneously with MIT just below the Fermi energy.

U-dependent Spectral Density at n=4/3 & 5/3



- 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 Li_xNbO2 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.