Creating and Tuning Electronic states, and Phases of NdNiO$_3$

Workshop on New Horizons in Quantum Correlated Materials
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Creation and Control of the electronic properties of $\text{ABO}_3$

**Distortion of the BO$_6$ octahedron**
- Energy splitting of the $d_{xy}$ & $d_{xz}$ & $d_{yz}$ bands

**Doping (through A)**
- Filling of the bands

**Octahedral rotations, Binding angles**
- Hopping probability, Effective mass
- Band width

**Proximity effects**
- Doping via charge transfer, Inducing orders (magnetism superconductivity...)

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**How to turn the knobs?**

- Defect Engineering;
- Altering crystal structure;
  - Lattice strain,
  - Proximity
  - ...

https://news.vanderbilt.edu
The modular system at the SIS beamline (ARPES+ PLD+STM+MBE) for developing functional materials with novel quantum properties
The new beamline at SLS 2.0

**QUEST (QUantum matter Electron Spectroscopy Tool)**

- **2 end stations** –
  - **ULTRA**: low temperature, high resolution + spin detection.
  - **OPERA** end station: complex systems, operando, micro-focus.

- **Advanced sample preparation.**
  methods: PLD, MBE,…

- **Complementary instrumentation**
  STS, STM, AFM.
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overview and motivation

$$t \equiv \frac{(\text{RE} - \text{O})}{\sqrt{2}(\text{Ni} - \text{O})}$$

0.7 < t < 9: orhtorombic, (Ni–O) bonds **under a tensile stress**
Tuning MIT in NdNiO$_3$ via strain and “dimensionality”

- **External pressure**
  
  ![Graph showing resistance vs. temperature for NdNiO$_3$ under different pressures.](image)


- **Strain and thickness (in NdNiO3 thin films)**
  
  ![Graphs showing resistivity vs. temperature for NdNiO$_3$ under different strain conditions.](image)

Tuning MIT in LaNiO$_3$ via “dimensionality”/thickness: ARPES view

E. Cappelli et al., APL Mater. 8, 051102 (2020)

Tuning MIT in NdNiO$_3$ via strain: What does happen?

NdNiO$_3$ on NGO (110) and LAO (100)

Tuning MIT in NdNiO$_3$ via strain: What happens?

FS at Z point

FS at Gama

R. Dhaka, MR et al., PRB 2015
Tuning MIT in NdNiO₃ via strain: What does happen?

Tensile strain: +1.4%

Compressive strain: -0.3%

20K Insulator phase NO FS

The momentum dependent density fluctuations (MRDF) modeling

Tuning MIT in NdNiO$_3$ via strain: What does happen?

NNO/NGO: Tensile strain

- Reduces MIT: 150 K compared to the bulk value of 200K
- Electronic structure: roughly the same as calculated for the untrain system


NNO/LAO: Compressive strain

- Significantly reduces MIT (50 K)
- Electronic structure: much different than calculated for the untrain system:
  - $e_g$ orbitals are lowered and
  - $t_{2g}$ orbitals are lifted.
  - The new, hole like, Fermi surface at A point.
ReNiO$_3$-Creating and Tuning Electronic states, and Phases

![Diagram showing phase transitions and magnetic properties of ReNiO$_3$.](image-url)
Tuning PHASE transition in NdNiO$_3$ Films via a Magnetic Underlayer

LSMO ground state FM-M
$T_c^{\text{BULK}} \approx 350$ K

LCMO ground state AFM-I/CO
$T_{\text{CO}}^{\text{BULK}} \approx 280$ K

M. Caputo, Z. Ristic et al., Adv. Sci., 8, 2101516, 2021
Tuning PHASE transition in NdNiO$_3$ Films via a Magnetic Underlayer

M. Caputo, Z. Ristic et al., Adv. Sci., 8, 2101516, 2021
Tuning PHASE transition in NdNiO$_3$ Films via a Magnetic Underlayer: ARPES view

M. Caputo, Z. Ristic et al., Adv. Sci., 8, 2101516, 2021
Momentum Dependent Density Fluctuations Modeling

M. Caputo, Z. Ristic et al., Adv. Sci., 8, 2101516, 2021
Tuning of ELECTRONIC states…

…and Creating the new PHASE of NdNiO₃