PAUL SCHERRER INSTITUT

PSI

Milan Radovic::Paul Scherrer Institute

Creating and Tuning Electronic states, and Phases of $NdNiO_3$

Workshop on New Horizons in Quantum Correlated Materials
ICTP-SAIFR, São Paulo, Brazil
August 15-19, 2022

Creation and Control of the electronic properties of ABO_3

Distortion of the BO_6 octahedron

Energy splitting of the d_{xy} & d_{xz} & d_{yz} bands

Doping (trough A)

Filling of the bands

Octahrdral rotations, Binding angles

Hopping probability, Effective mass Band width

Proximity effects

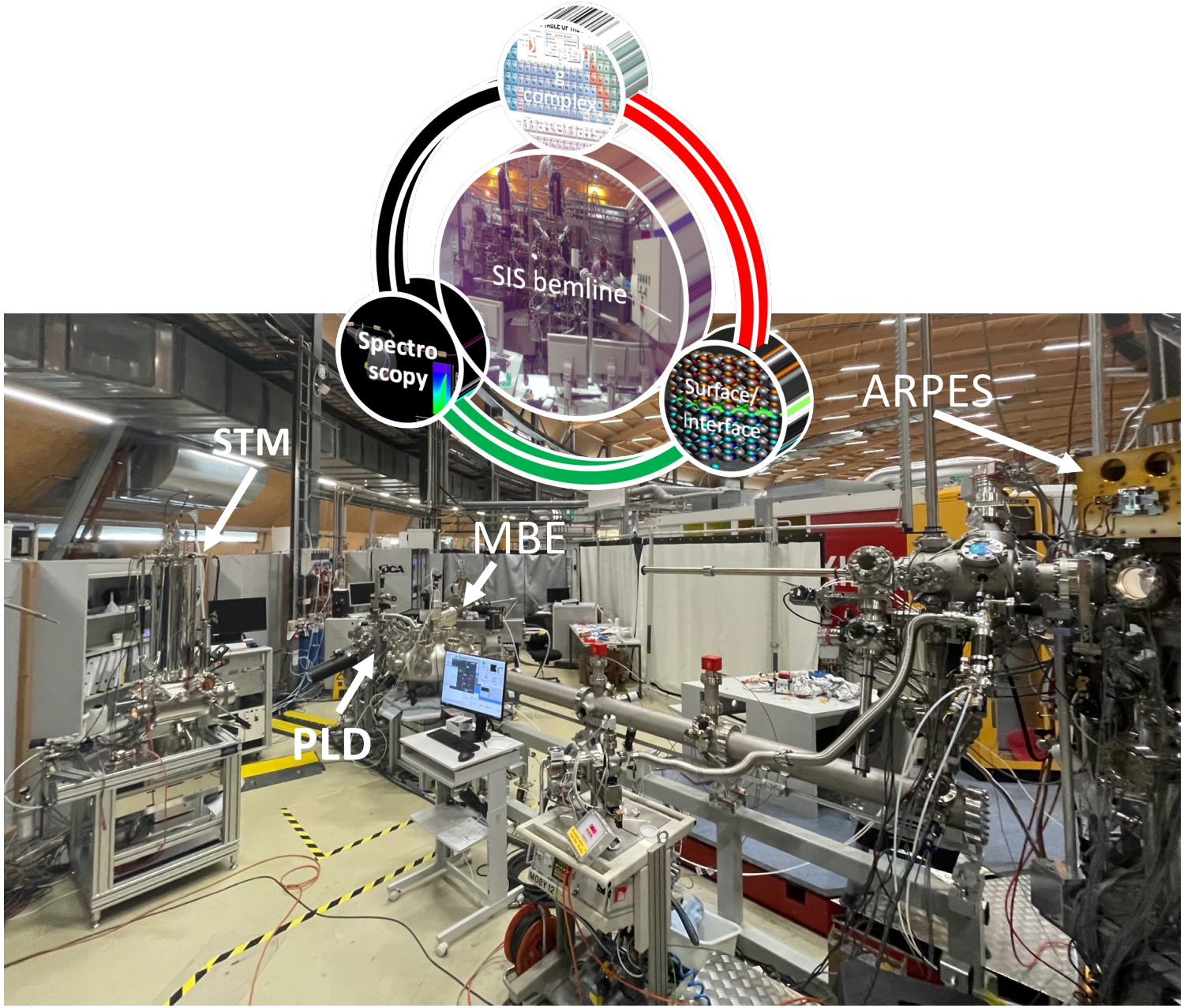
Doping via charge transfer, Inducing orders (magnetism superconductivity…)

How to turn the knobs?

- ✓ Defect Engineering;
- ✓ Altering crystal structure;
- ✓ *Lattice strain,*
- ✓ *Proximty*
- ✓ …

https://news.vanderbilt.edu

The modular system at the SIS beamline (ARPES+ PLD+STM+MBE) for developing functional materials with novel quantum properties

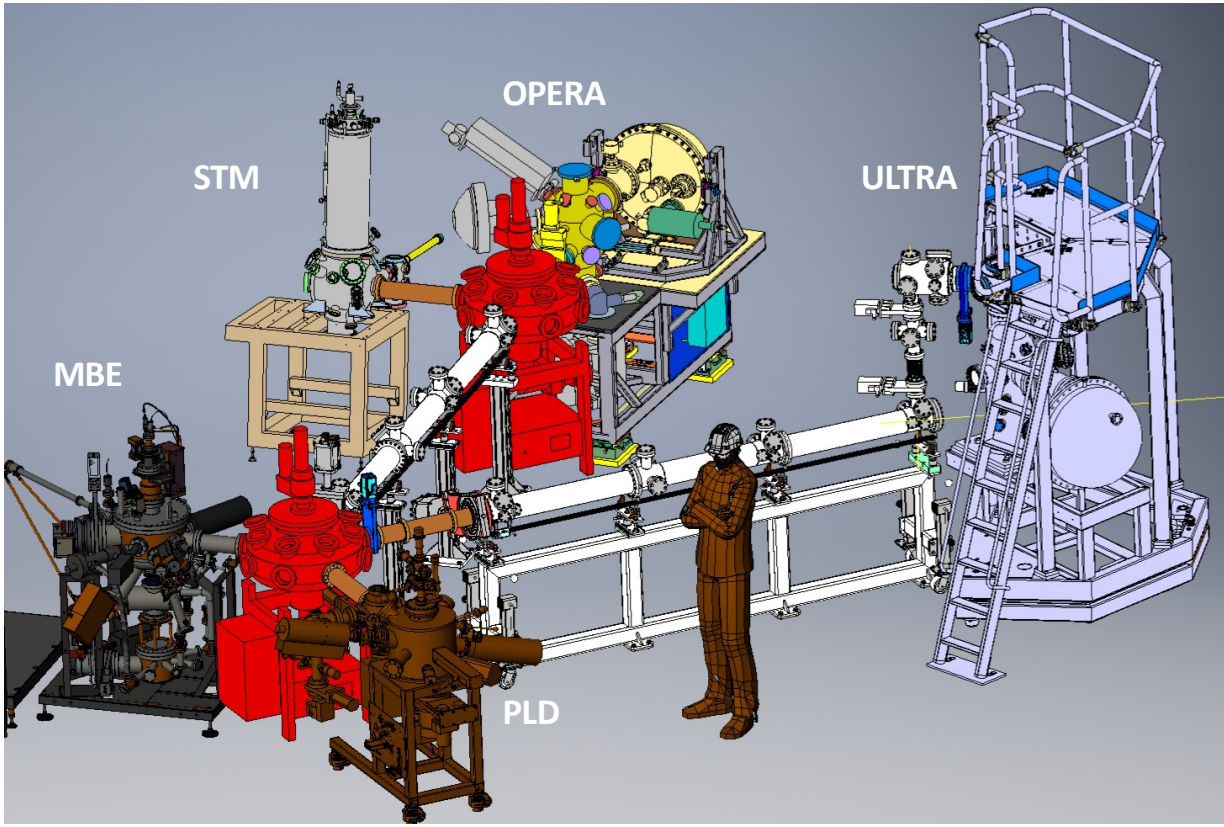


The new beamline at SLS 2.0

QUEST (QUantum matter Electron Spectroscopy Tool)

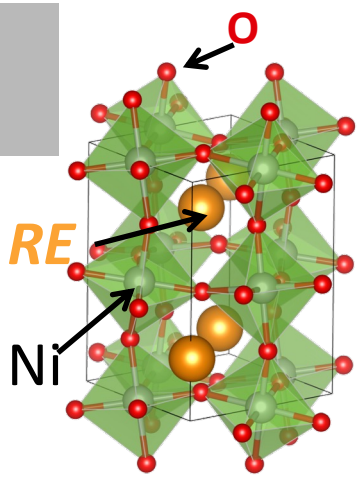
M. Muntwiller, T. Jung, M. Shi, T. Schmitt, N. Plumb, M.R.

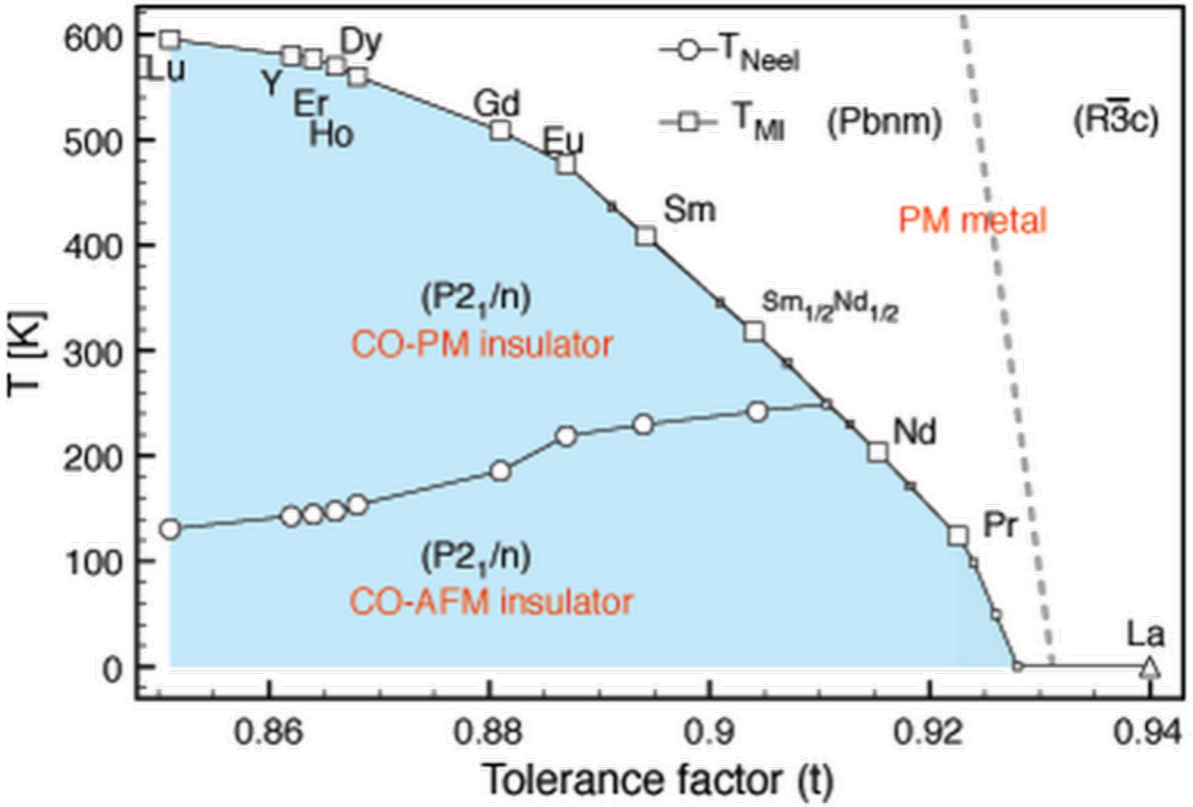
- **2 end stations** –
  - **ULTRA**: low temperature, high resolution + spin detection.
  - **OPERA** end station: complex systems, operando, micro-focus.
- **Advanced sample preparation.** methods: PLD, MBE,…
- **Complementary instrumentation** STS, STM, AFM.



Creating and Tuning Electronic states, and Phases of $NdNiO_3$

overview and motivation





bond length

$$t \equiv (RE–O)/\sqrt{2}(Ni–O)$$

bond length

0.7 <t < 9: orhtorombic,
(Ni–O) bonds ***under a tensile stress***

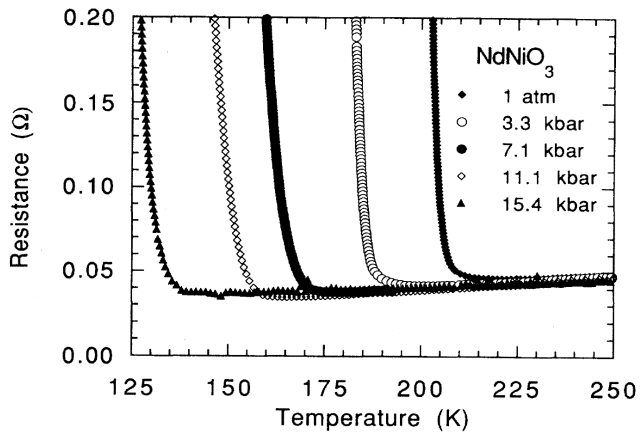
John B. Goodenough * and J.-S. Zhou J. Mater. Chem., 2007, **17**, 2394-2405

M.L. Medarde, J. Phys.: Condens. Matter 9 (1997) 1679–1707

*http://dpmc.unige.ch/gr_triscone/research.php?topic=nickelates

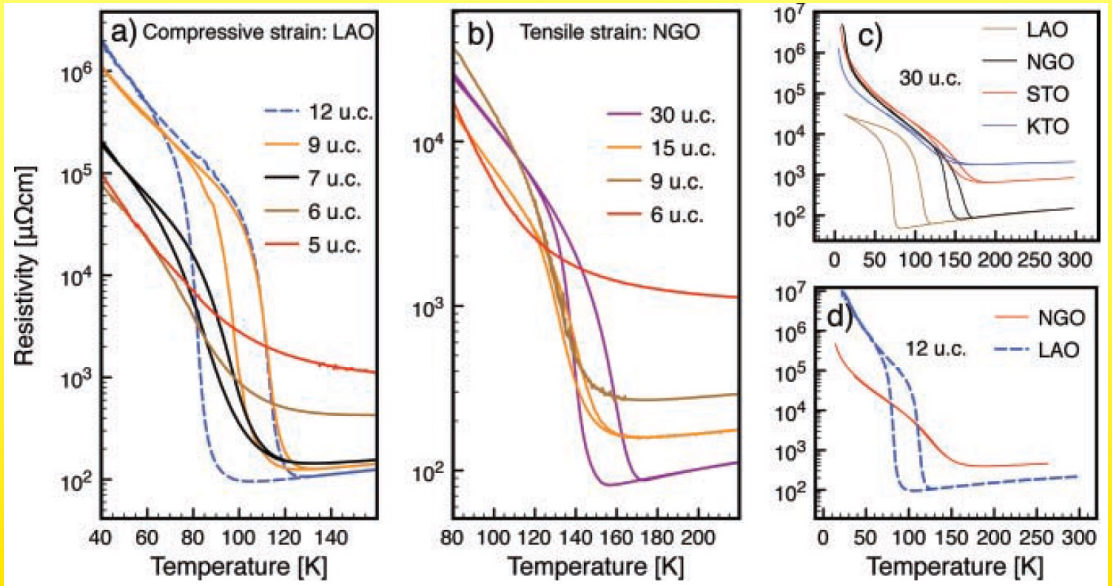
Tuning MIT in $NdNiO_3$ via strain and "dimensionality"

- **External pressure**



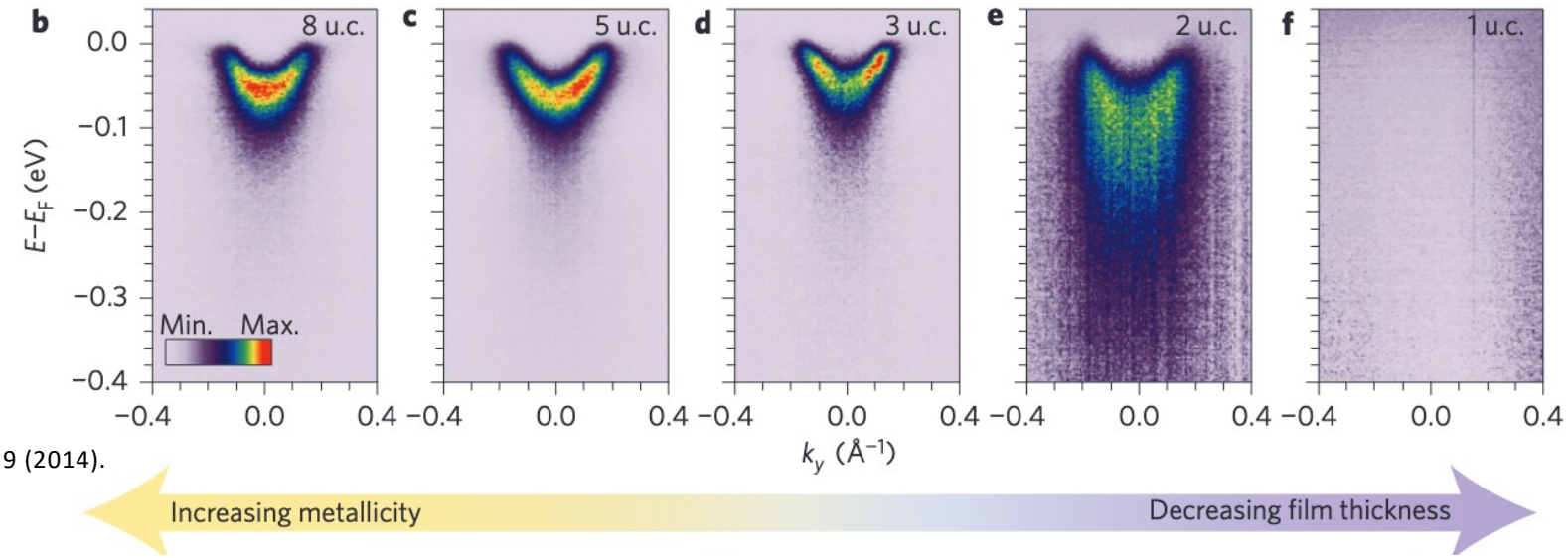
X. Obradors et al., Phys. Rev. B 47, 12353, 1993.

- **Strain and thickness (in NdNiO3 thin films)**

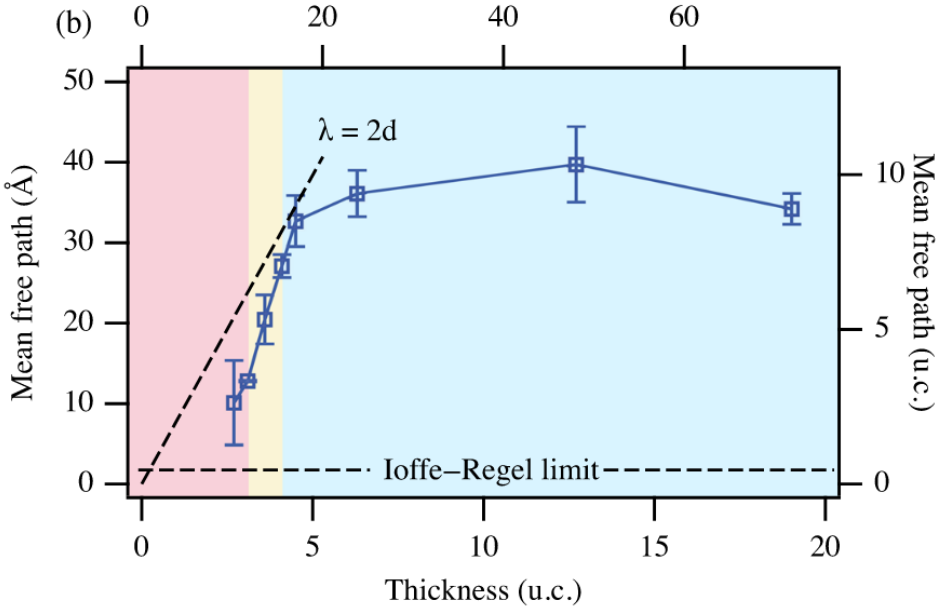


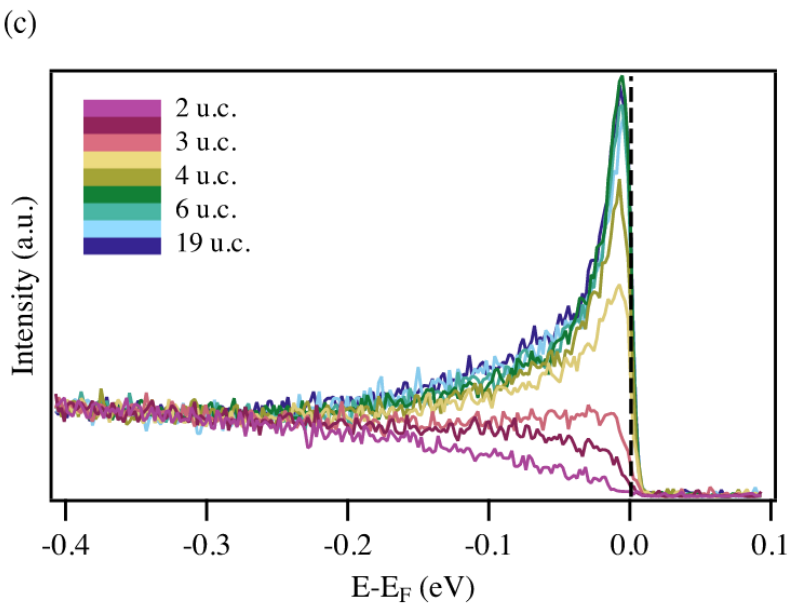
R. Scherwitzl at al;Adv. Mater. 22, 5517–5520, 2010

Tuning MIT in $LaNiO_3$ via "dimensionality"/thickness: ARPES view



P. D. C. King et al.,
Nature Nanotech. 59, Vol 9 (2014).

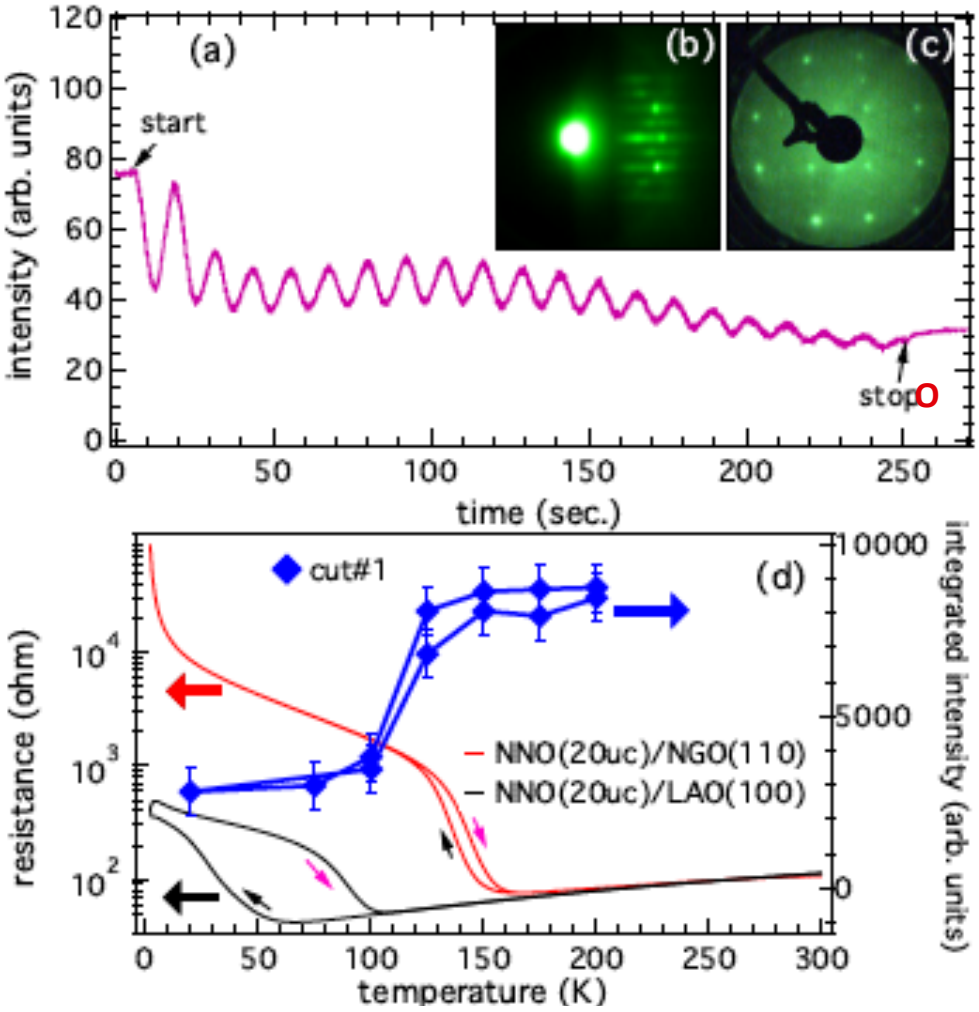




E. Cappelli et al., APL Mater. 8, 051102 (2020)

Tuning MIT in $NdNiO_3$ via strain: What does happen?

$NdNiO_3$ on NGO (110) and LAO (100)

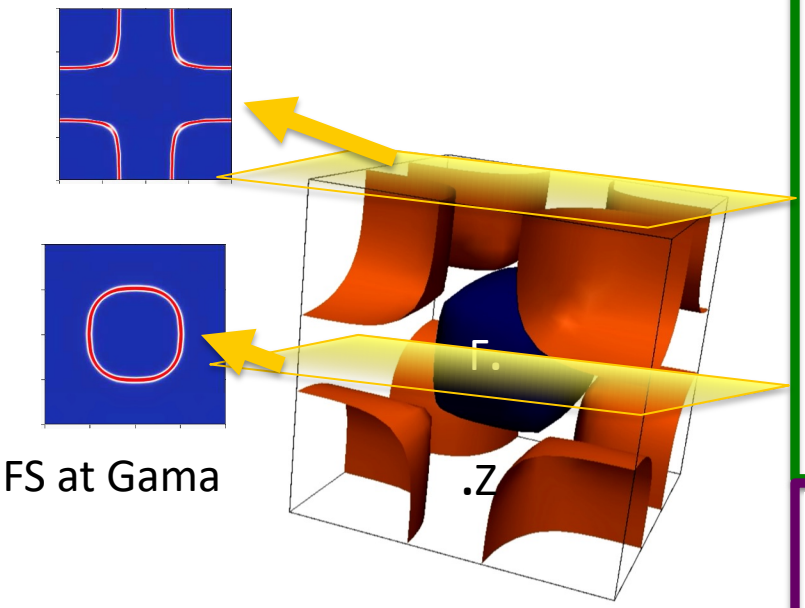


t_{2g}

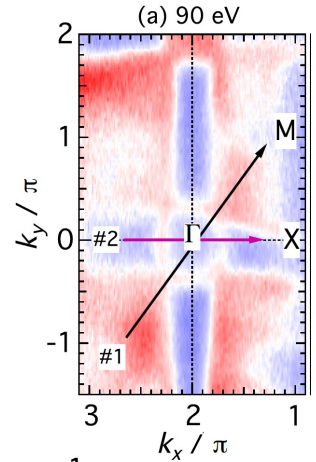
R. Dhaka, et al., Phys. Rev. B 92, 035127, *2015*

Tuning MIT in $NdNiO_3$ via strain: What happens?

FS at Z point



FS at Gama

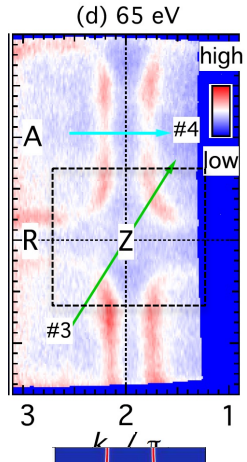


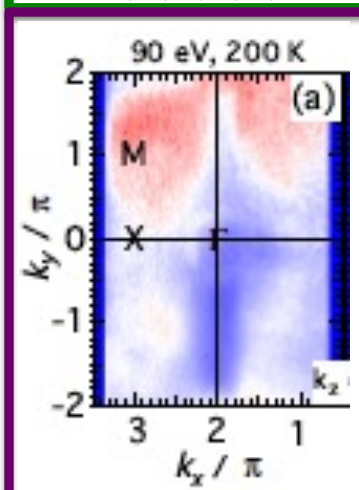
200 K

Tensile strain: + 1.4%

NNO /20 u.c./

NGO(110)



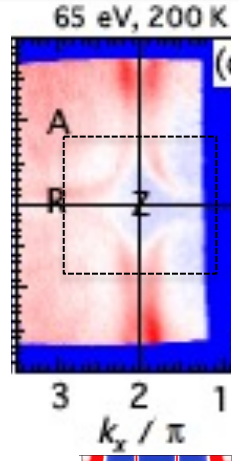


200 K

Compressive strain: -0.3%

NNO /20 u.c./

LAO(100)



R. Dhaka, MR et al., PRB 2015

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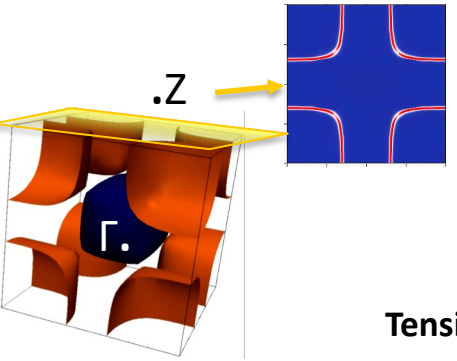
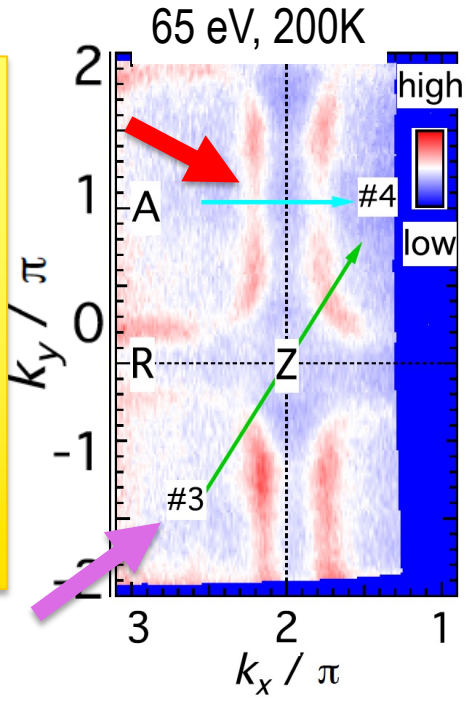
Tuning MIT in $NdNiO_3$ via strain: What does happen?



Tensile strain: + 1.4%

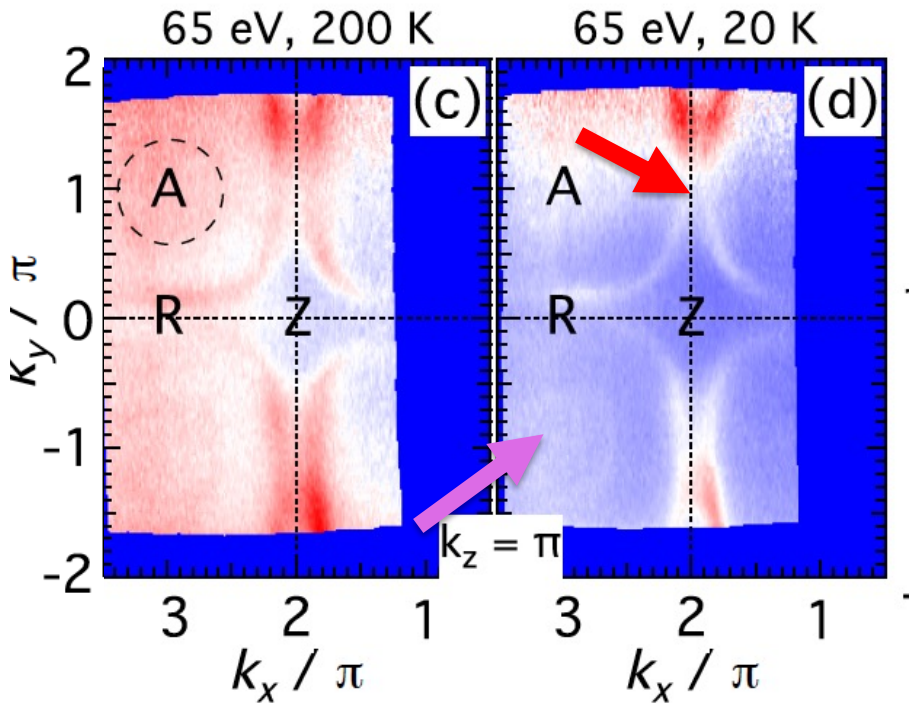
NNO /20 u.c./
NGO(110)

20K Insulator phase NO FS



Compressive strain: -0.3%

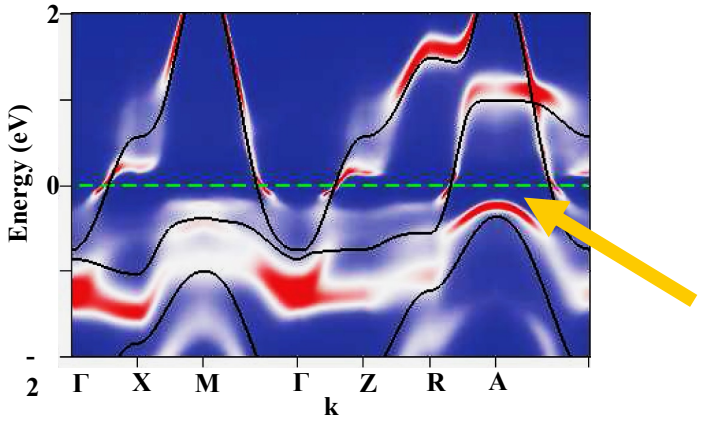
NNO /20 u.c./
LAO(100)

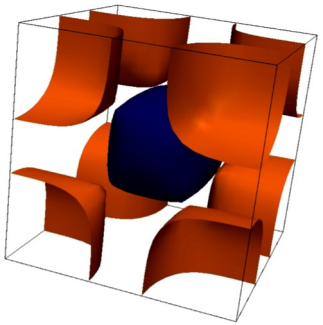


R. Dhaka, et al., Phys. Rev. B 92, 035127, *2015*

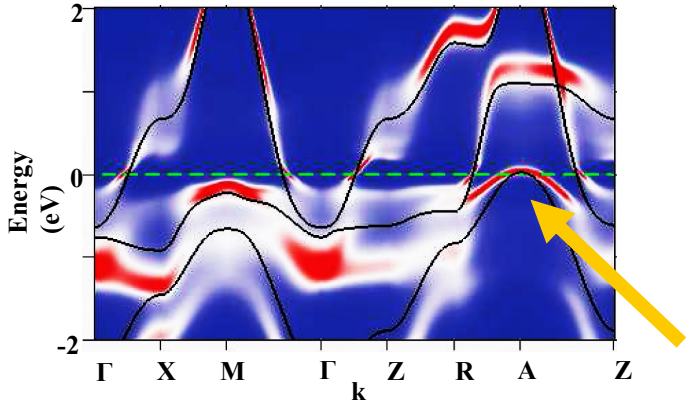
Tuning MIT in $NdNiO_3$ via strain: What does happen?

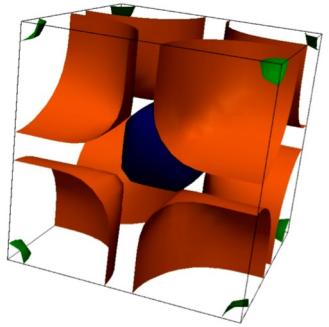
NNO/NGO: Tensile strain: + 1.4%





NNO/LAO: Compressive strain: -0.3%



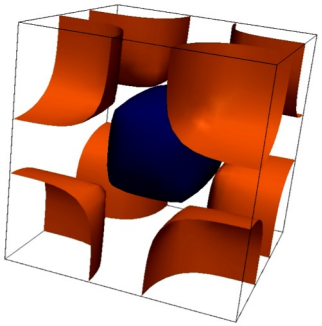


The momentum dependent density fluctuations (MRDF) modeling

R. Dhaka, et al., Phys. Rev. B 92, 035127, *2015*

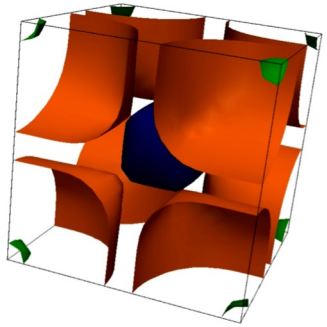
Tuning MIT in $NdNiO_3$ via strain: What does happen?

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

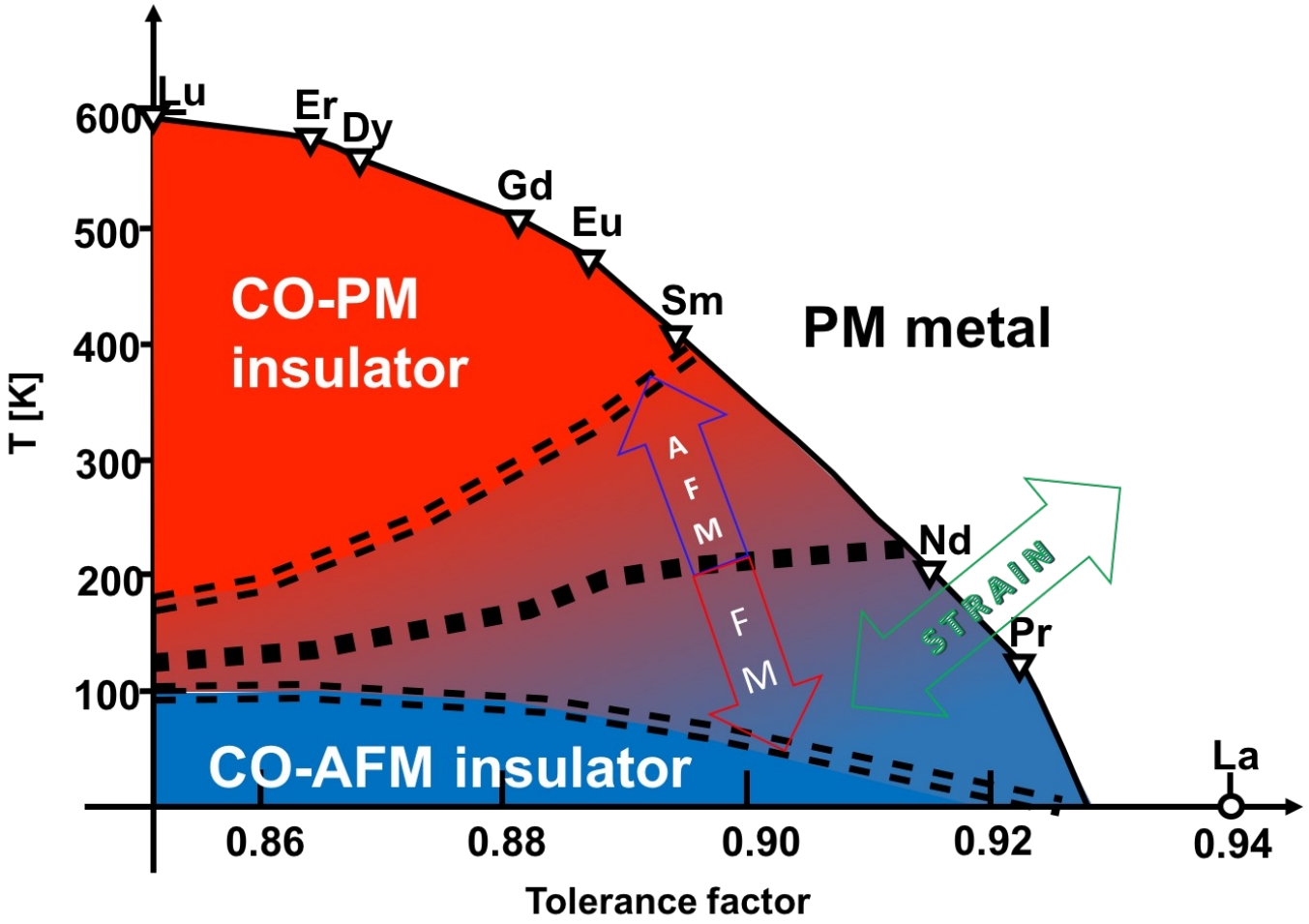
NNO/LAO: Compressive strain



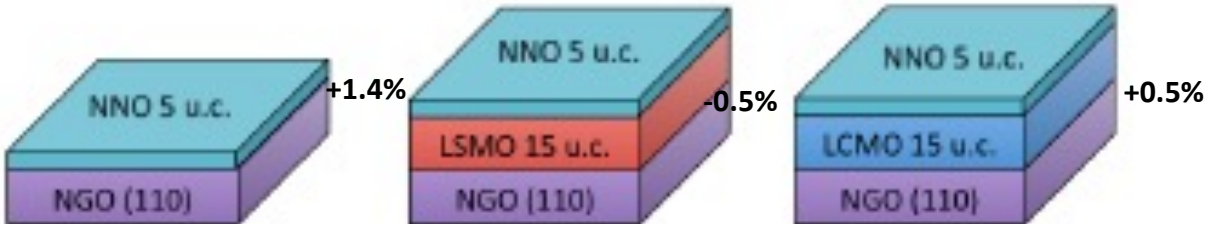
- Significantly reduces MIT (50 K)
- Electronic structure: much different than calculated for the untrain system:
  - e_g orbitals are lowered and
  - t_{2g} orbitals are lifted.
  - The new, hole like, Fermi surface at A point.

R. Dhaka, et al., Phys. Rev. B 92, 035127, *2015*

$ReNiO_3$-Creating and Tuning Electronic states, and Phases

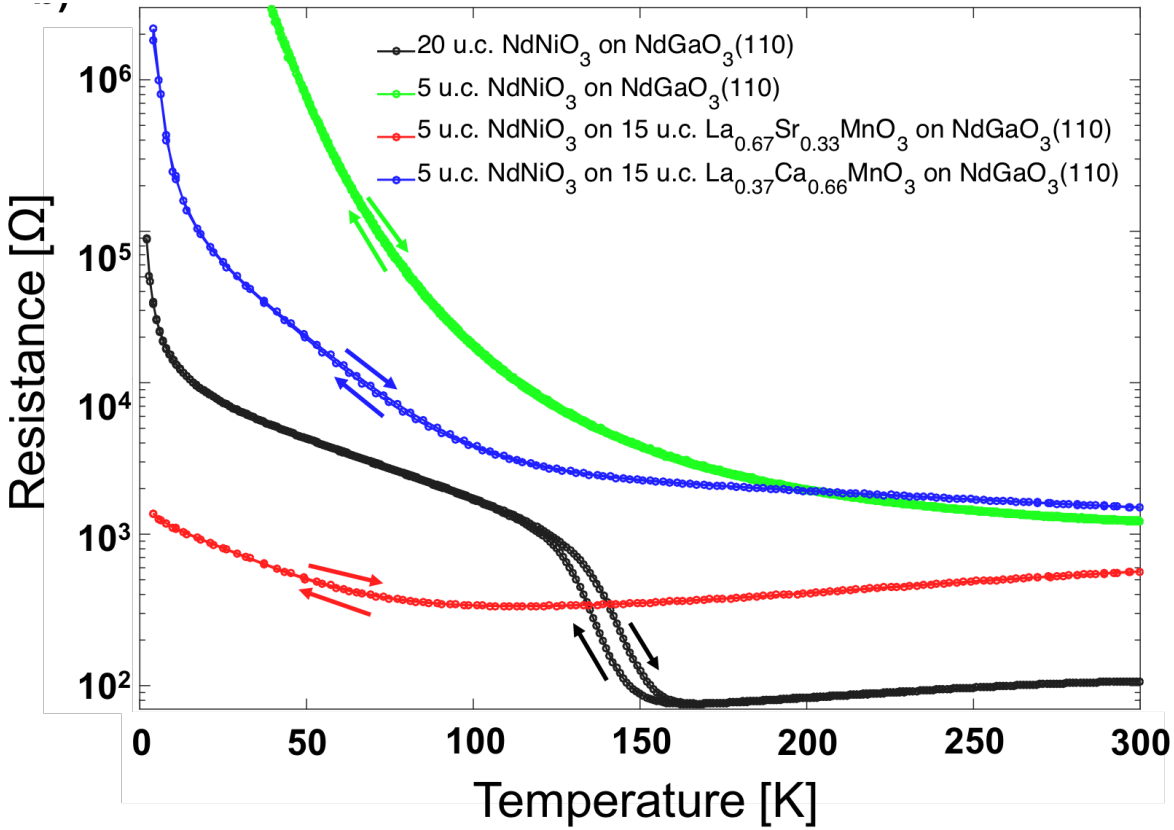


Tuning PHASE transition in $NdNiO_3$ Films via a Magnetic Underlayer



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

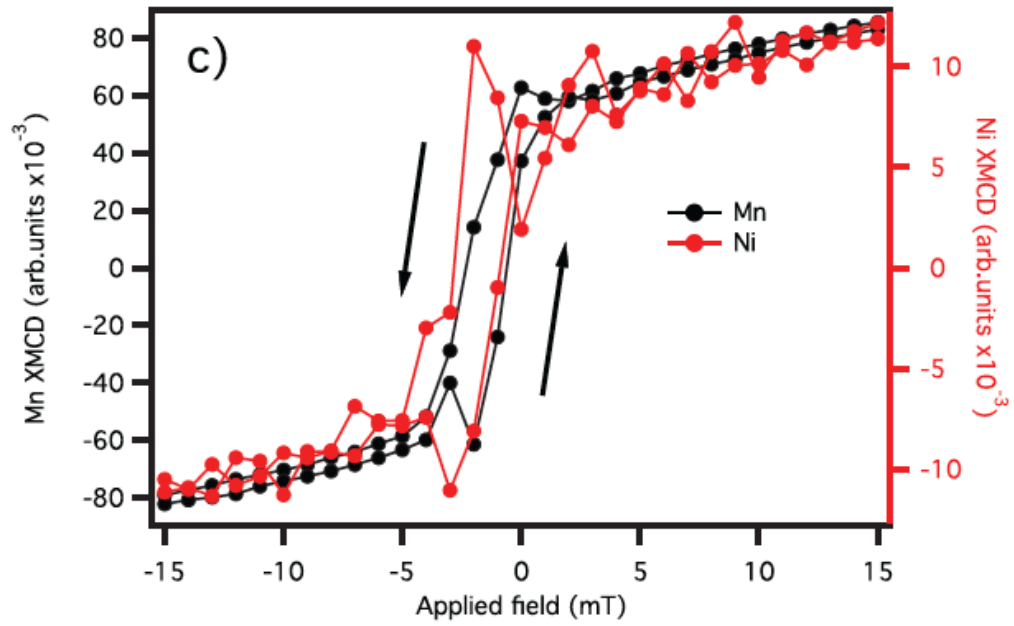
LCMO ground state AFM-I/CO
$T_{CO}^{BULK} \approx 280$K

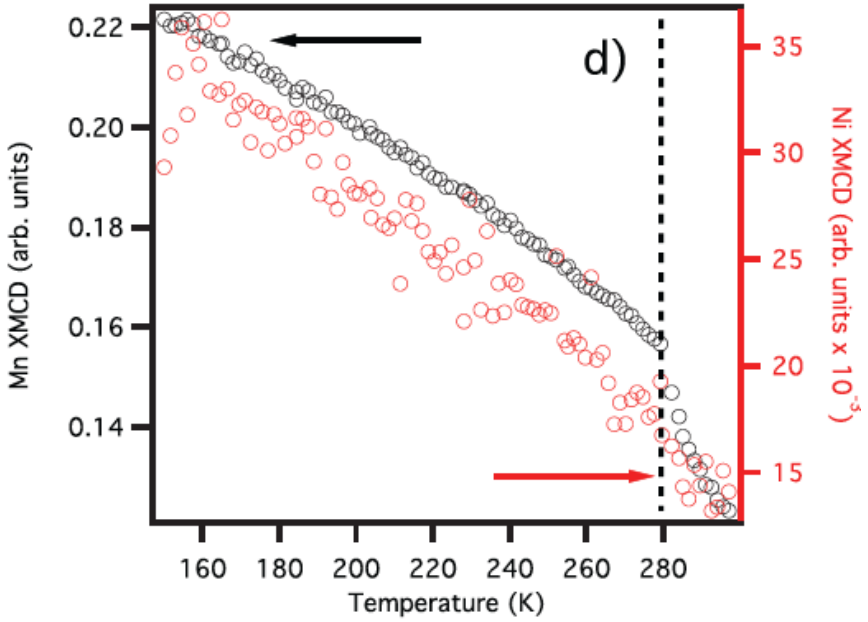


M. Caputo, Z. Ristic et al., Adv. Sci., 8, 2101516, 2021

Tuning PHASE transition in $NdNiO_3$ Films via a Magnetic Underlayer

NNO /5 u.c./
LSMO /15 u.c./
NGO(110)





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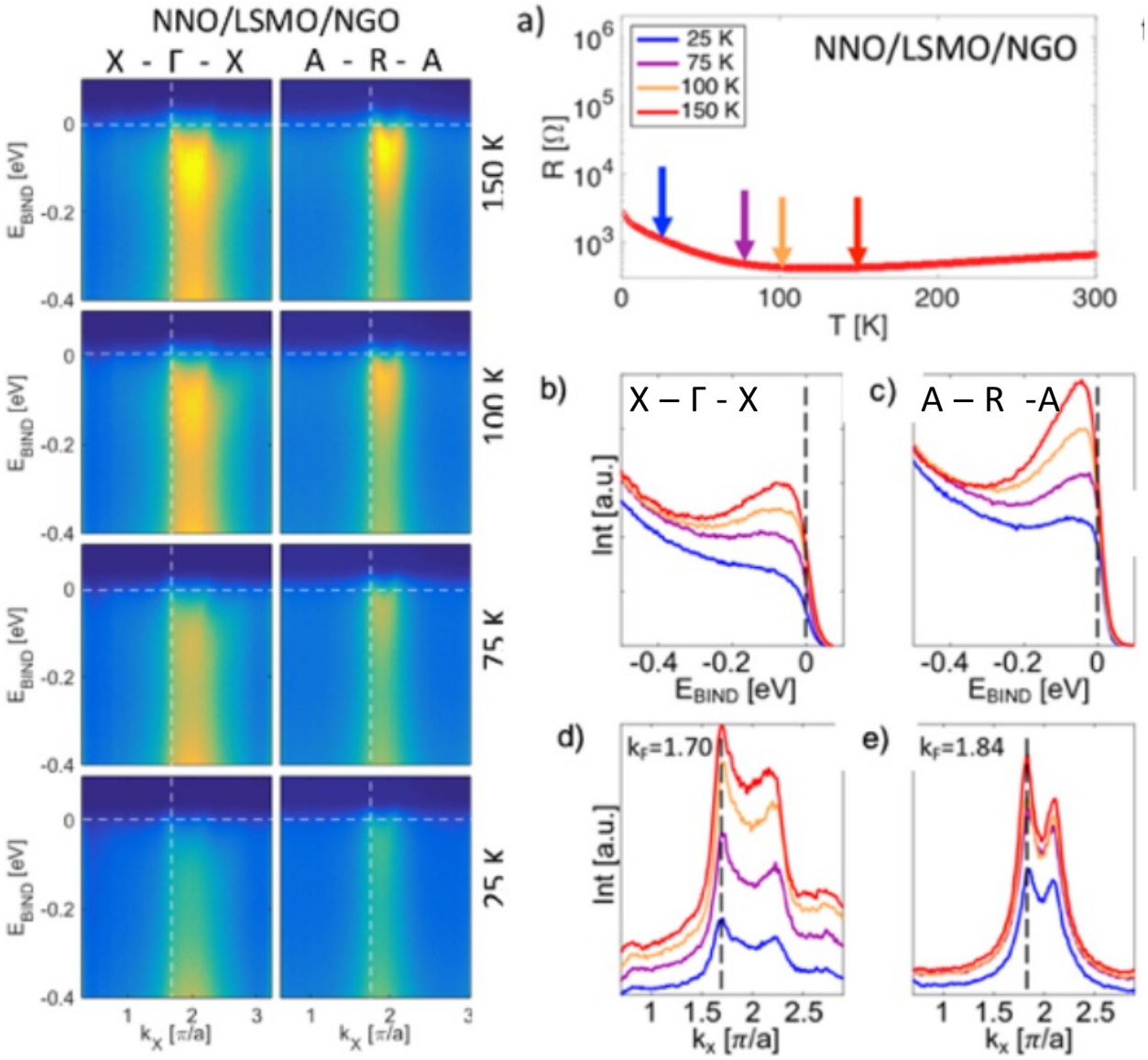
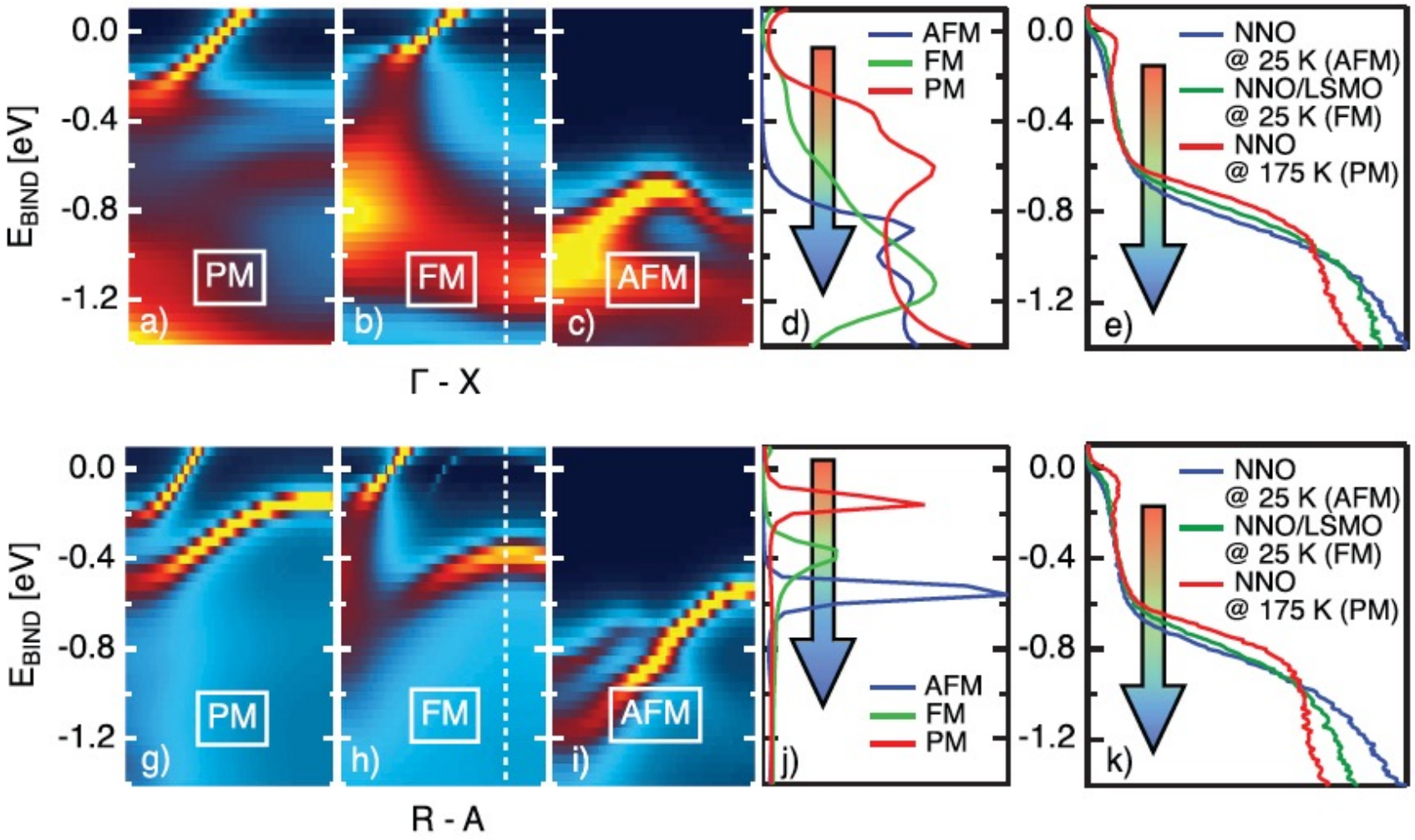
Tuning PHASE transition in $NdNiO_3$ Films via a Magnetic Underlayer: ARPES view



M. Caputo, Z. Ristic et al., Adv. Sci., 8, 2101516, 2021

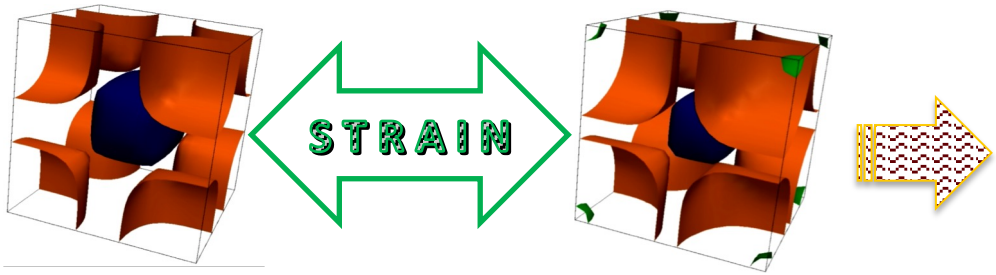
Tuning PHASE transition in $NdNiO_3$ Films via a Magnetic Underlayer: ARPES view

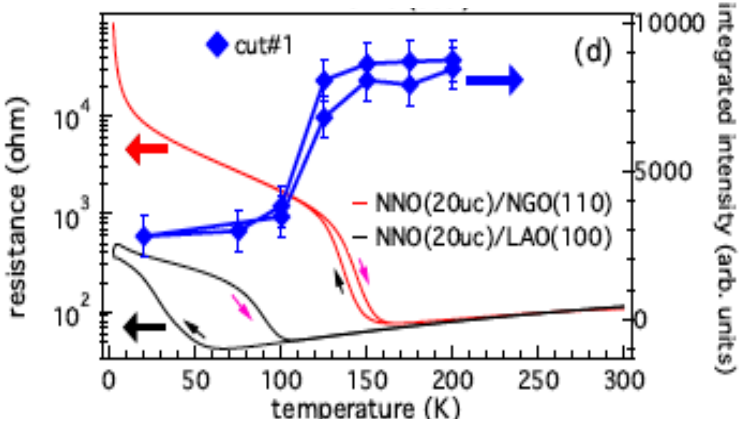
Momentum Dependent Density Fluctuations Modeling



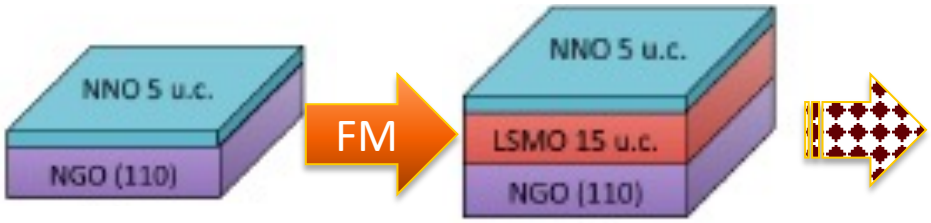
M. Caputo, Z. Ristic et al., Adv. Sci., 8, 2101516, 2021

Tuning of ELECTRONIC states…





…and Creating the new PHASE of $NdNiO_3$



XMCD on 5.u.c. NNO/FM-Manganites