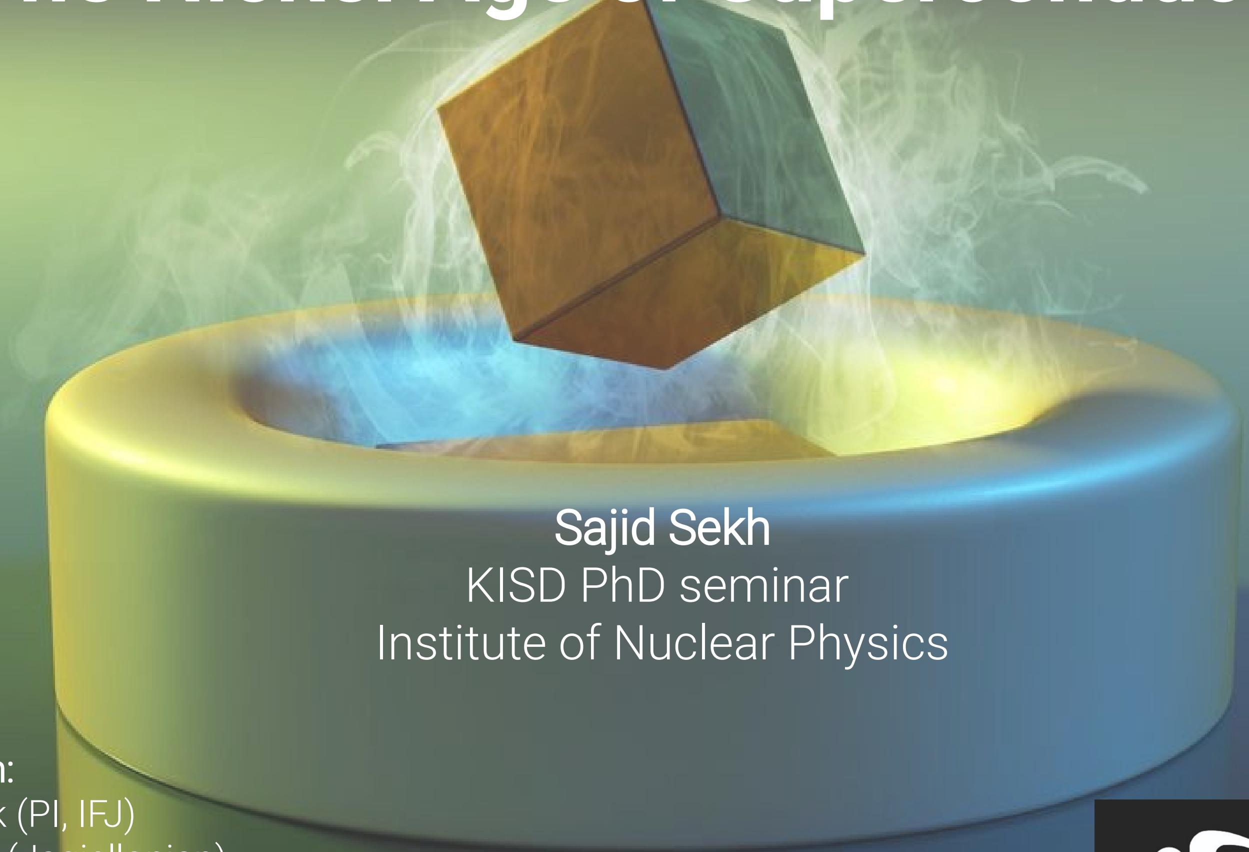
22 March, Krakow

The Nickel Age of Superconductivity



Sajid Sekh
KISD PhD seminar
Institute of Nuclear Physics

Team:
Andrzej Ptok (PI, IFJ)
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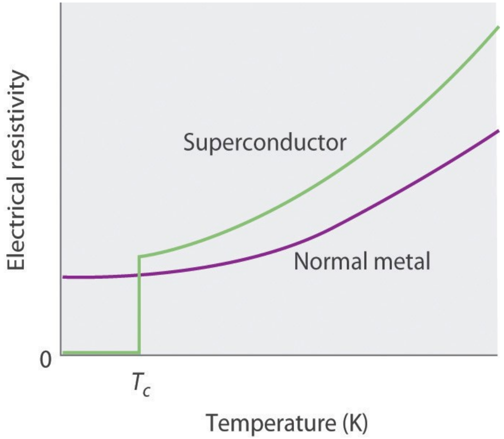
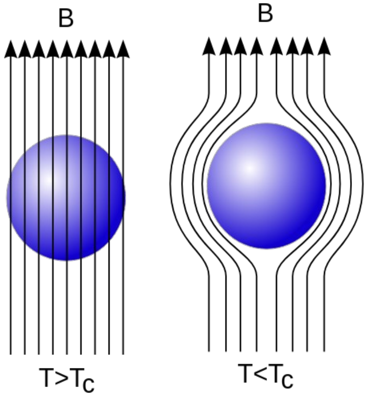
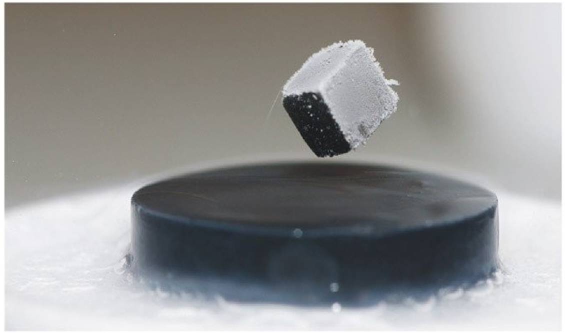
Przemyslaw Piekarz (IFJ) ,
Andrzej M. Oles (Jagiellonian)

INSTYTUT FIZYKI JĄDROWEJ
IM. HENRYKA NIEWODNICZAŃSKIEGO
POLSKIEJ AKADEMII NAUK

Superconductivity



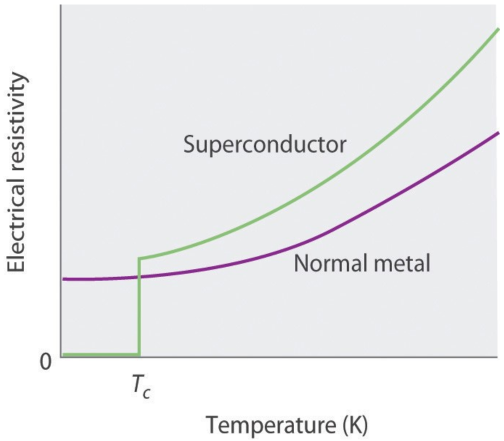


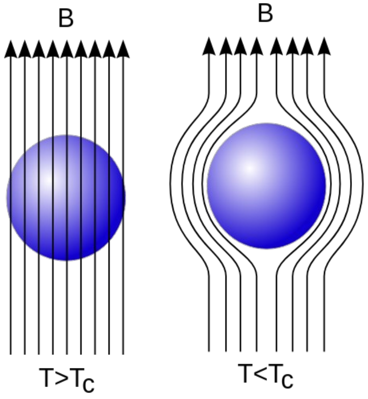


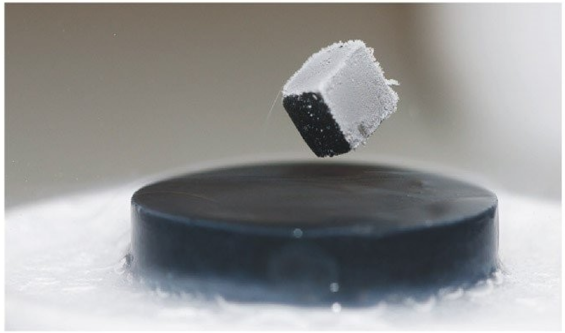
US Dept. of Energy

- Resistivity drops to zero below T_c
- Repulsion of magnetic fields (Meissner effect)

Superconductivity







US Dept. of Energy

- Resistivity drops to zero below T_c
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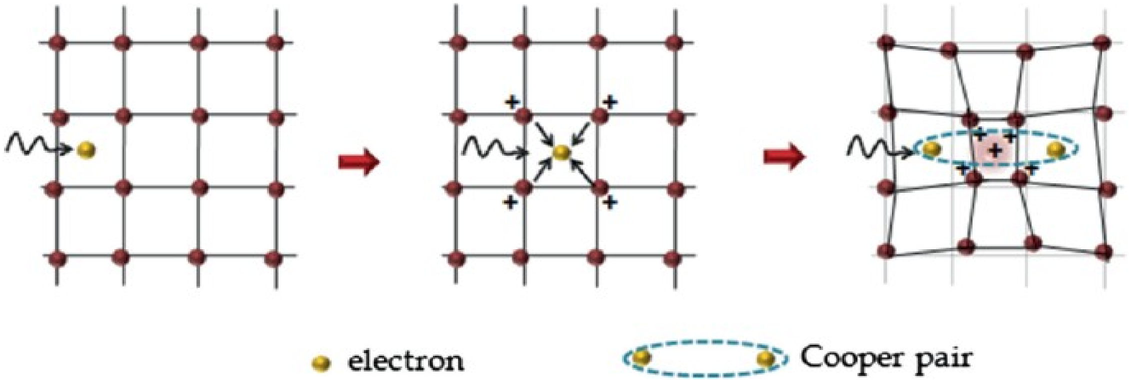
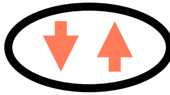
BCS theory of superconductivity

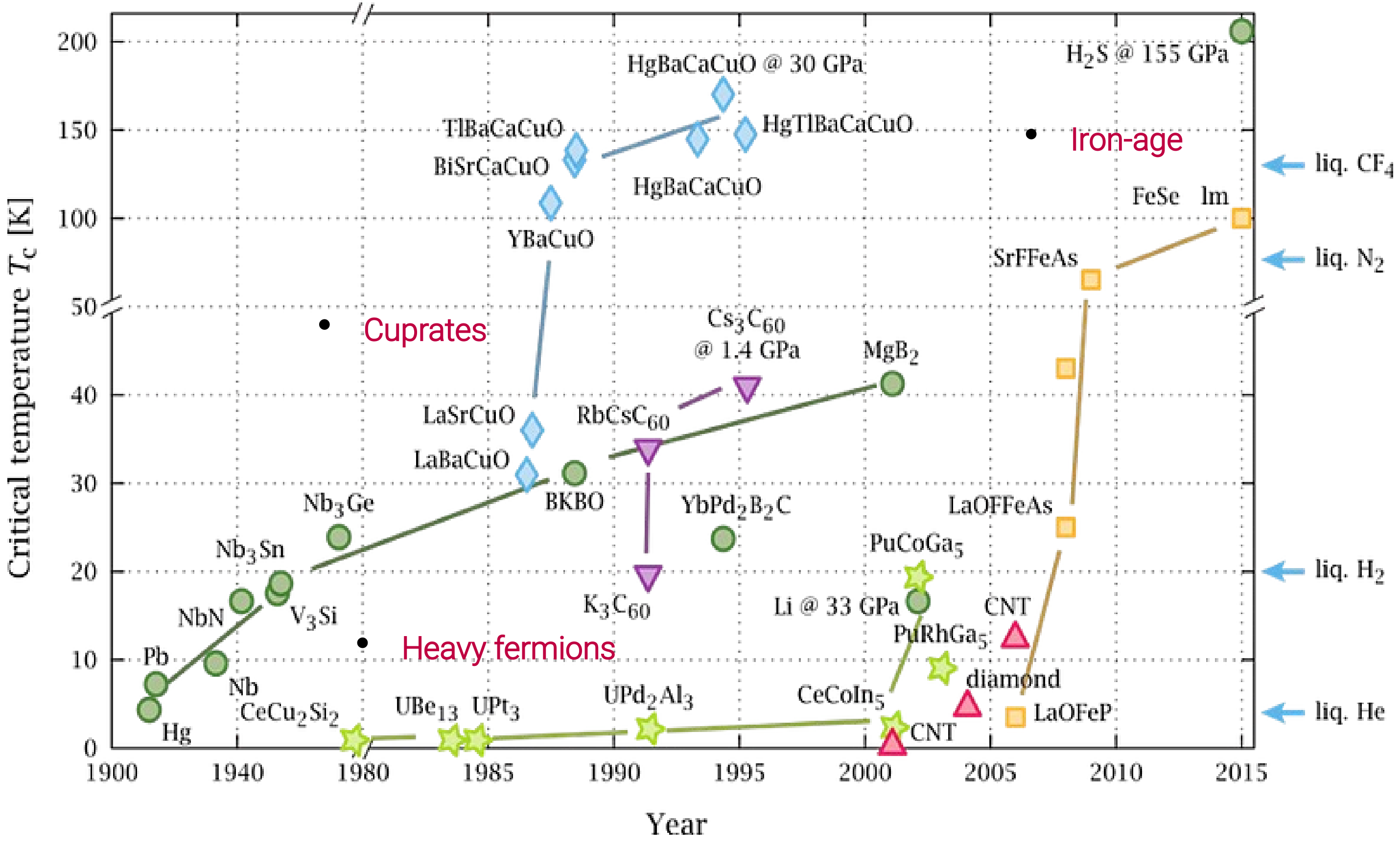


- Attractive interaction b/w electrons
- Pairing of opposite spins - Copper pairs



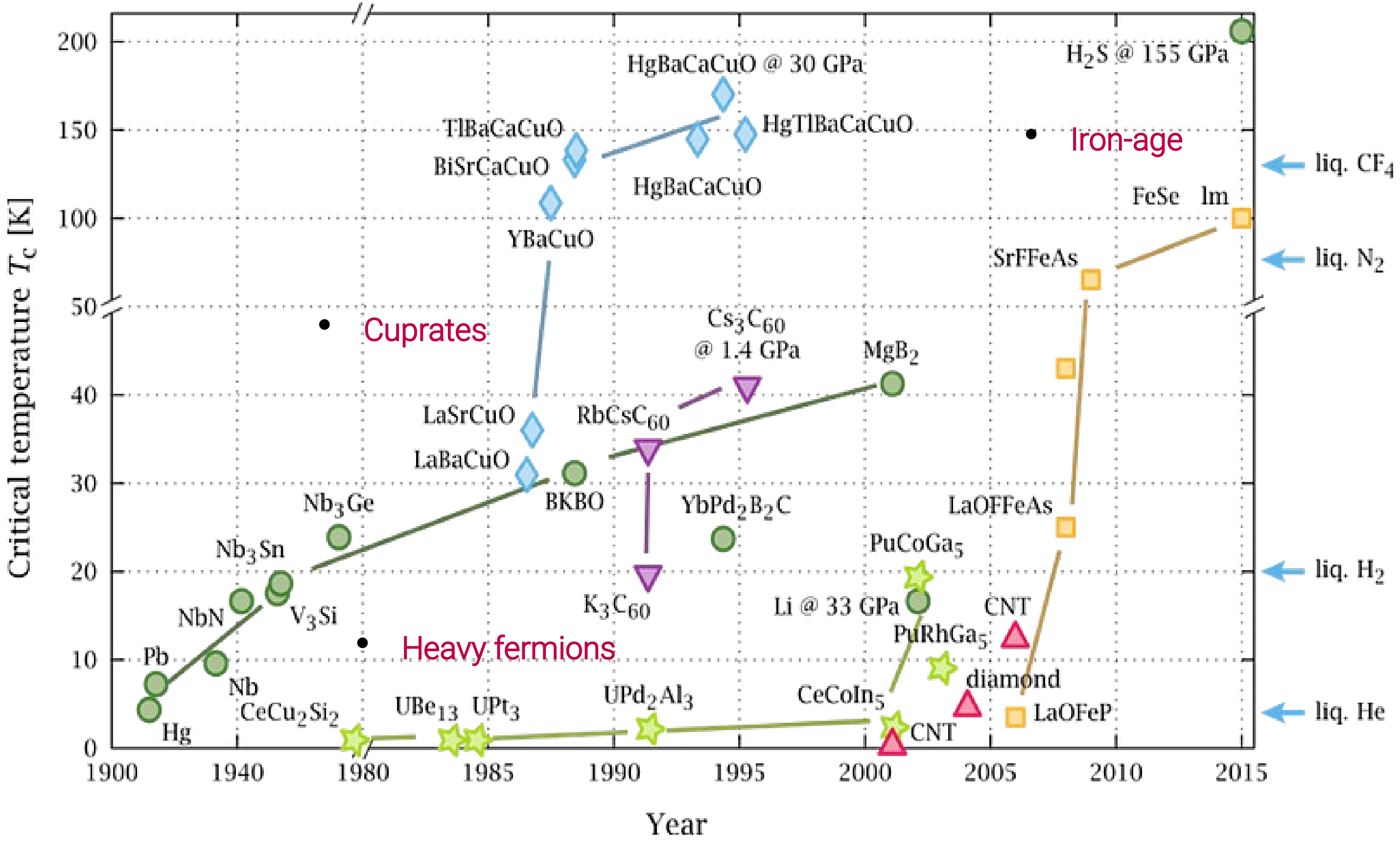
- T_c ~10K – not very useful

High-Tc superconductivity



Credits: Pia Jensen Ray, master thesis, Copenhagen 2016

High-Tc superconductivity



- <u>Application ($$):</u>
- Transport of energy without dissipation
- Can revolutionize several
- industries
- A Nobel prize

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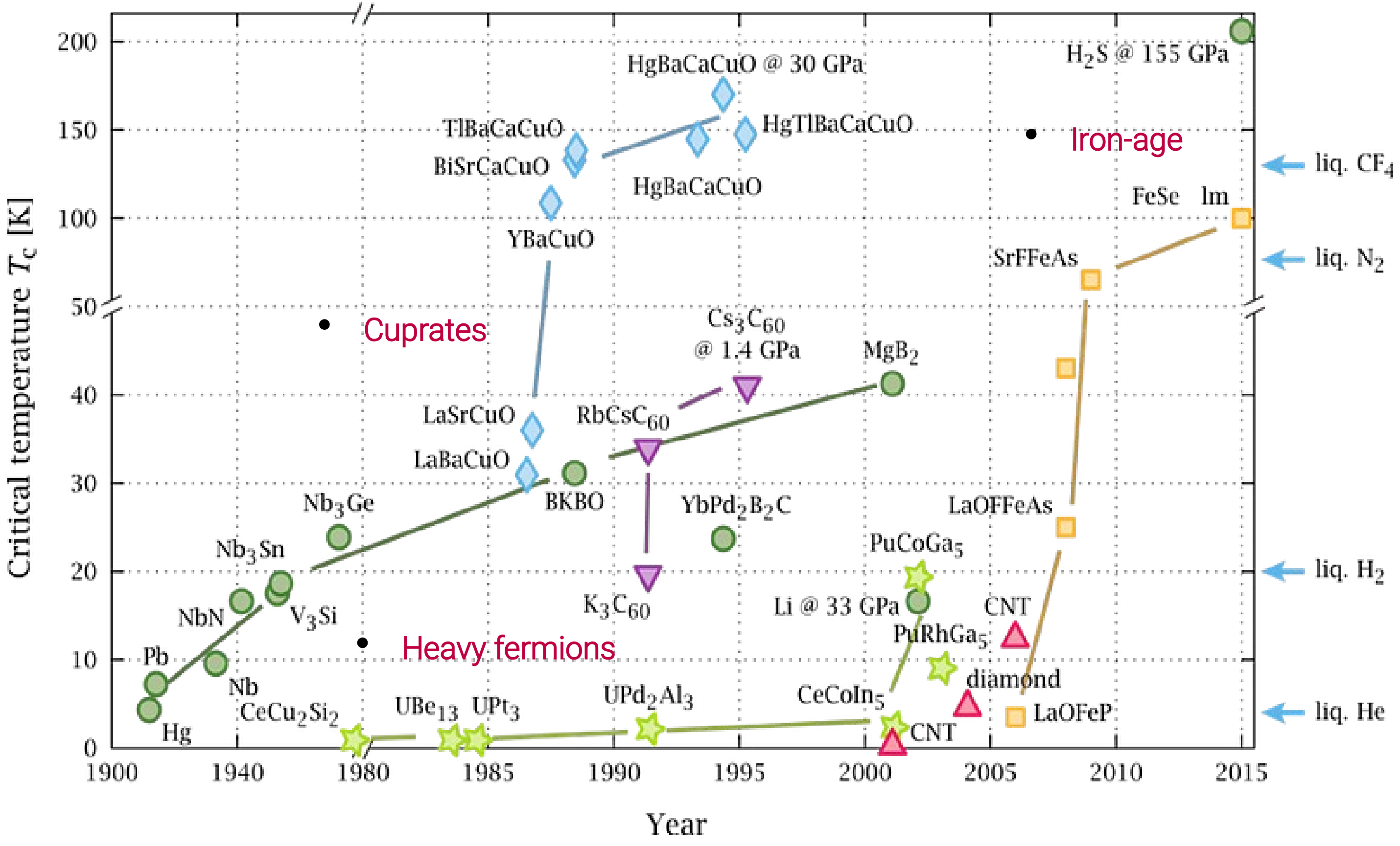
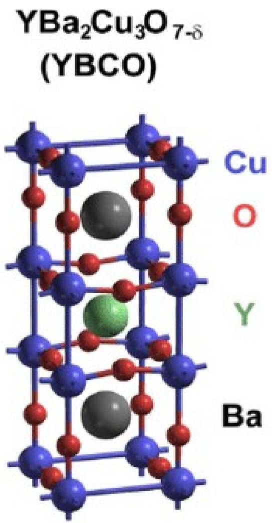
High-Tc superconductivity



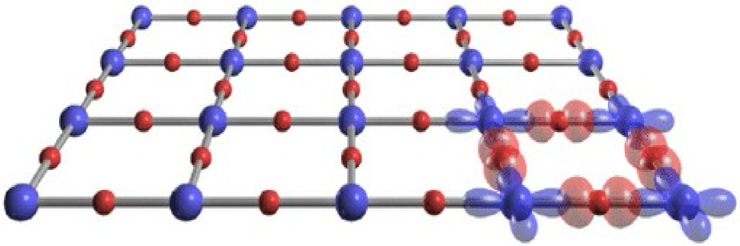
Credits: Pia Jensen Ray, master thesis, Copenhagen 2016

- Application ($$):
- Transport of energy without dissipation
- Can revolutionize several
- industries
- A Nobel prize
- Intellectual:
- Strongly interacting electrons – High Tc SCs provide nice test bed for toy models
- Rich and new electronic and magnetic properties

Cuprate superconductors

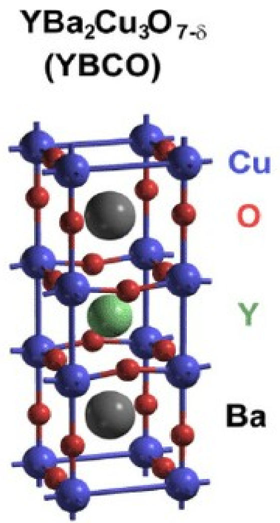


Layered structure

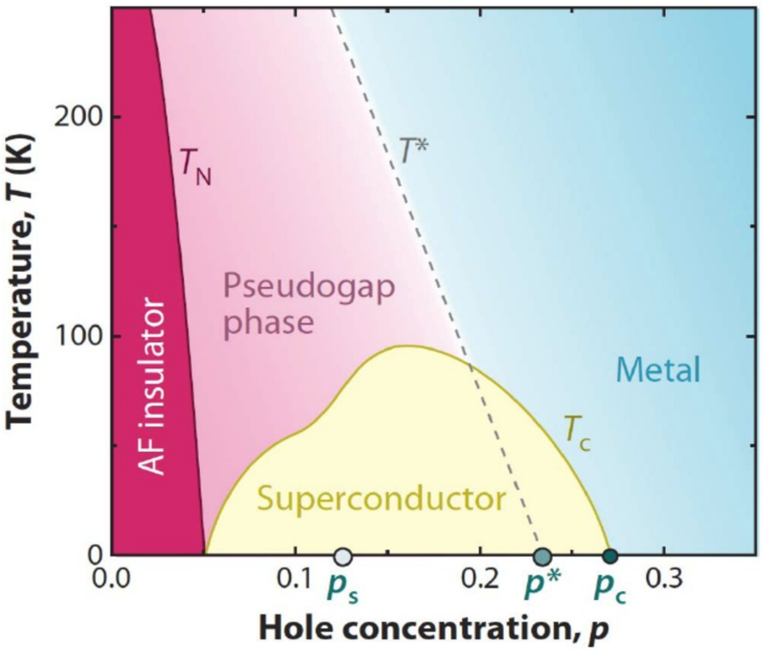


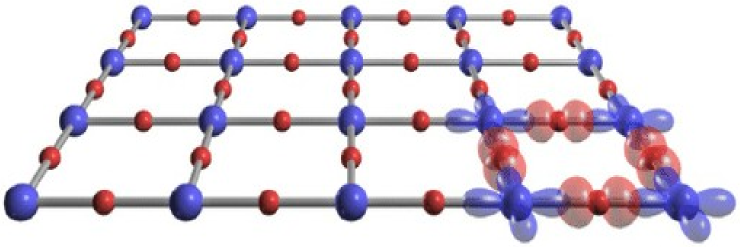
Square CuO_2 plane

Cuprate superconductors



Layered structure





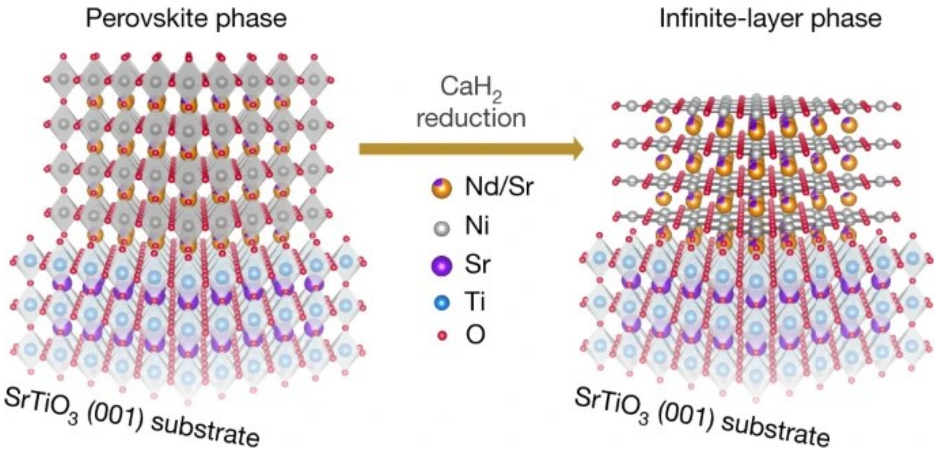
Square CuO_2 plane

Facts about Cuprates:

- ➔ Parent compound is an insulator
- ➔ Taking away electrons (hole doping) induces
- ➔ superconductivity
- ➔ Overdoping leads to a metal
- ➔ T_C can go up to 133K (-140C)
- ➔ Not described by BCS theory – new physics?

Taillefer et. al., Annual Review of CMP, 1:51-70
Barišić et. al., PNAS 110 (30) 12235

Nickel age of superconductivity

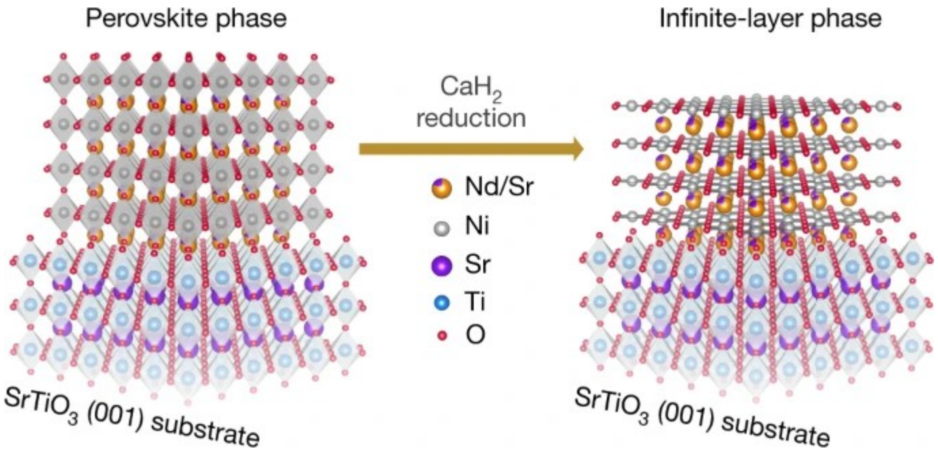


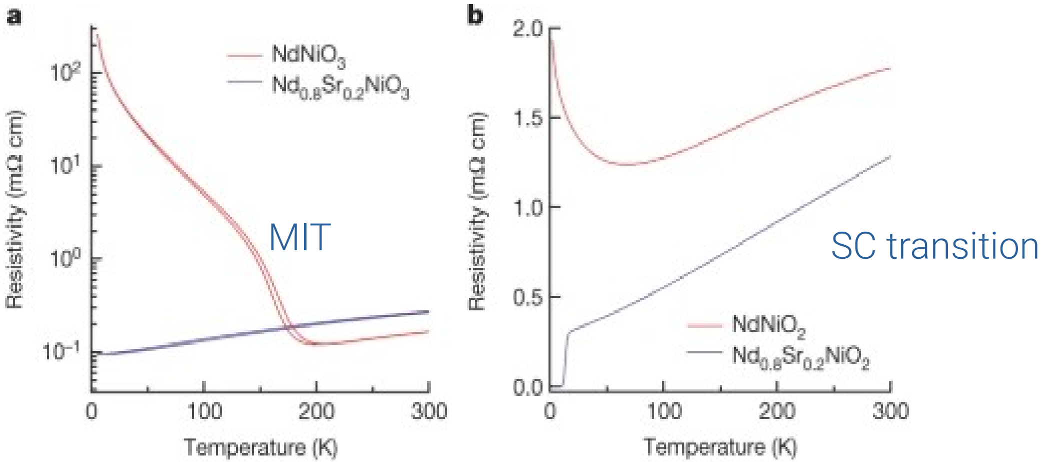
Perovskite: NdNiO3

Infinite-layer nickelate: NdNiO2

SC is only thin films, not in bulk!

Nickel age of superconductivity





Perovskite: NdNiO3

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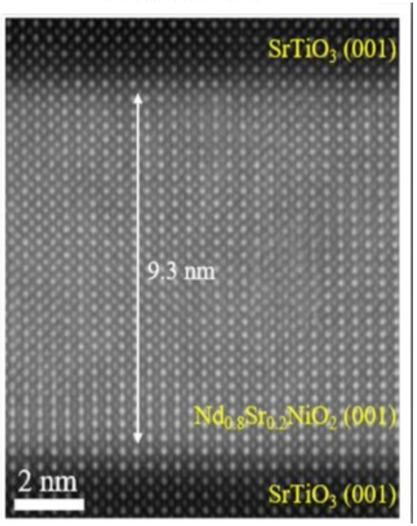


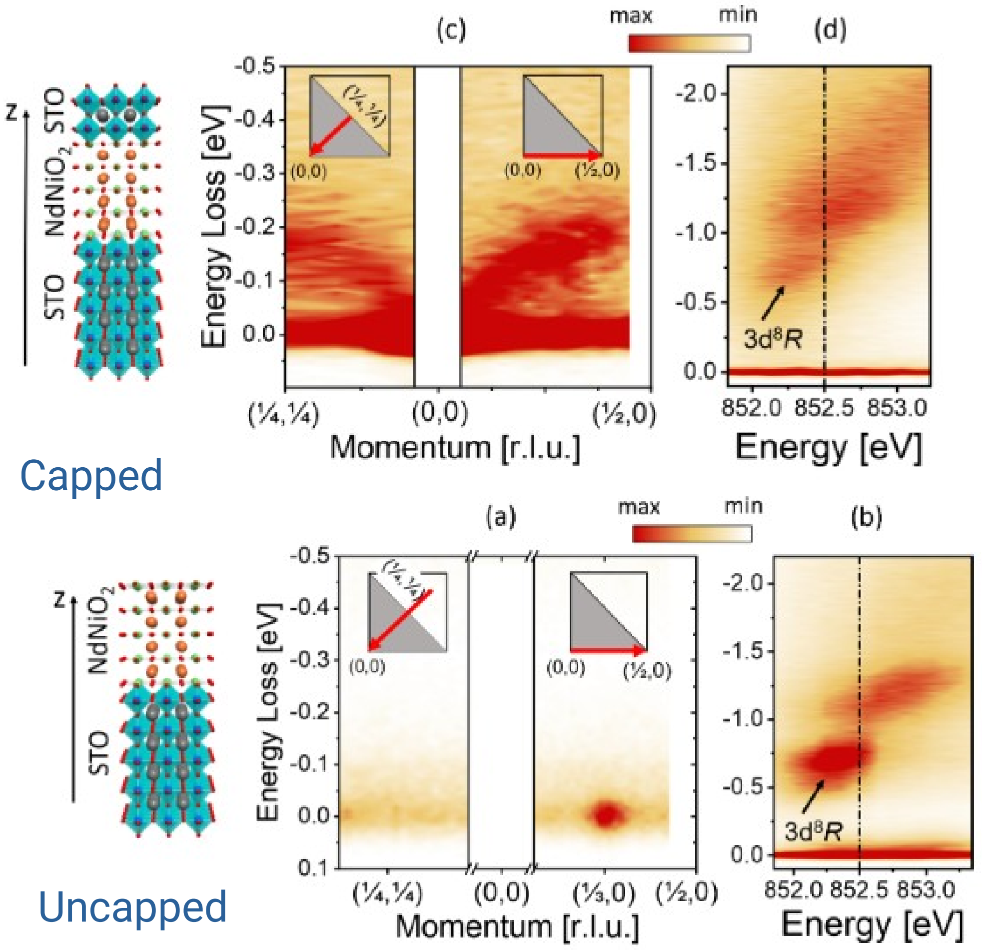
Superconductivity in an infinite-layer nickelate

Danfeng Li, Kyuho Lee, Bai Yang Wang, Motoki Osada, Samuel Crossley, Hye Ryoung Lee, Yi Cui, Yasuyuki Hikita & Harold Y. Hwang

Nature **572**, 624–627 (2019) | Cite this article

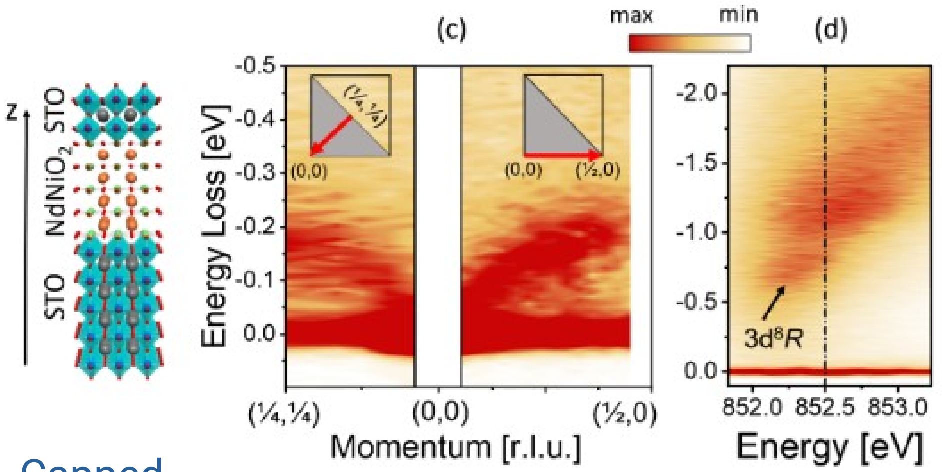
SC is only thin films, not in bulk!

Contrasting properties in thin films

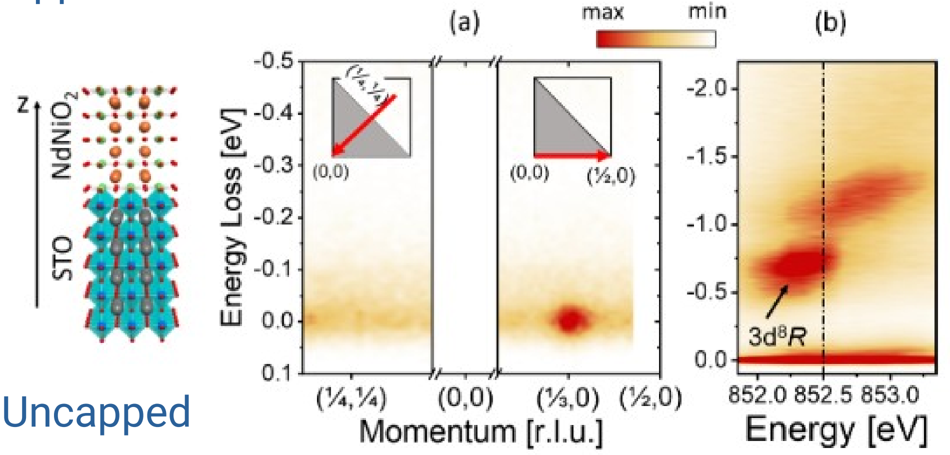


Rossi et al, Nat Phys, 18, 869 (2022)
Krieger et al, PRL, 129, 027002 (2022)
Tam et al, Nat Mater, 21, 1116 (2022)

Contrasting properties in thin films



Capped

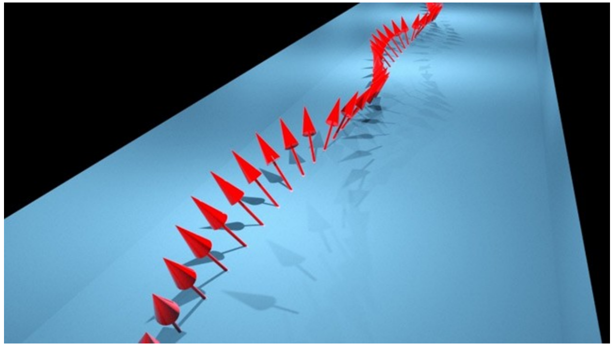


Uncapped

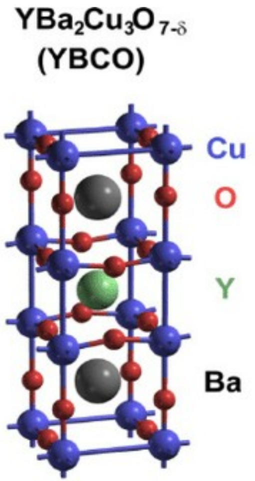
Rossi et al, Nat Phys, 18, 869 (2022)
Krieger et al, PRL, 129, 027002 (2022)
Tam et al, Nat Mater, 21, 1116 (2022)

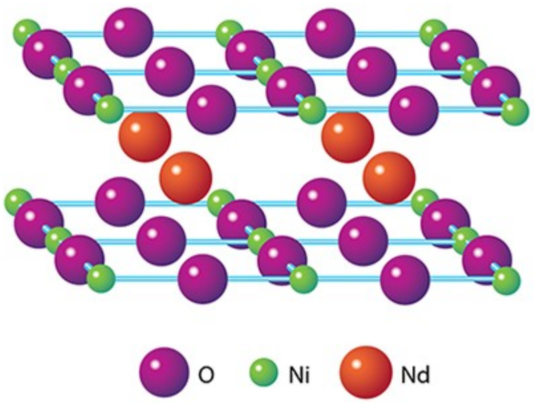
	Uncapped	Capped
Spin waves	No	Yes
Nd-Ni hybridization	Strong	Weak
Charge order	**Q**~(1/3,0)	No

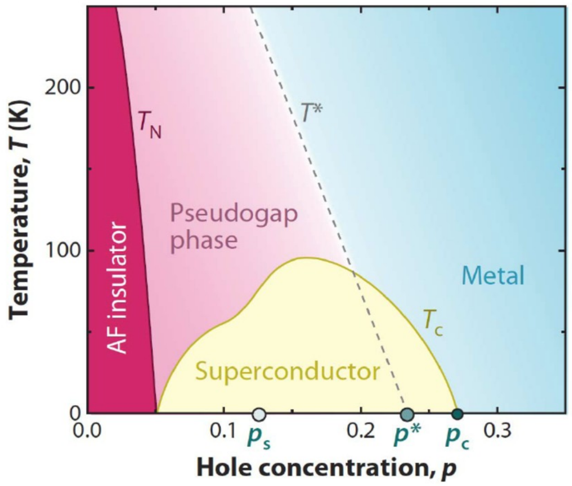
Spin waves

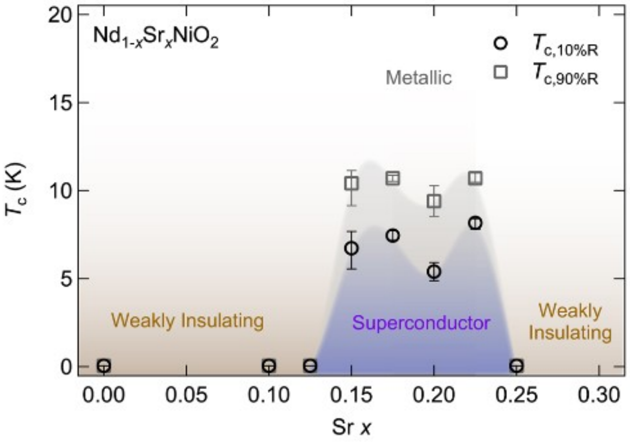


Cuprates vs. Nickelates



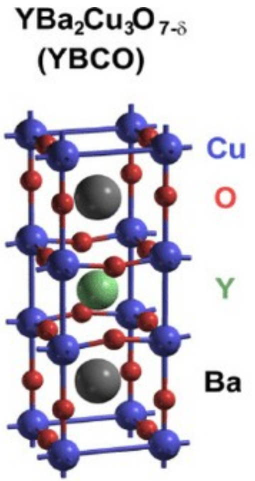


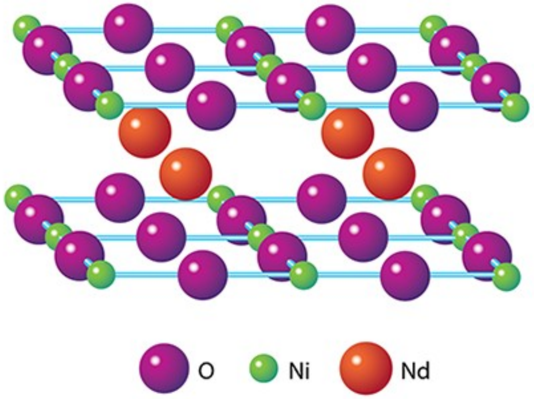


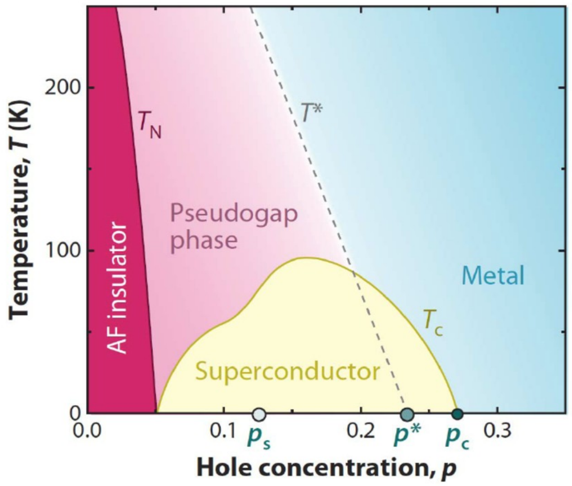


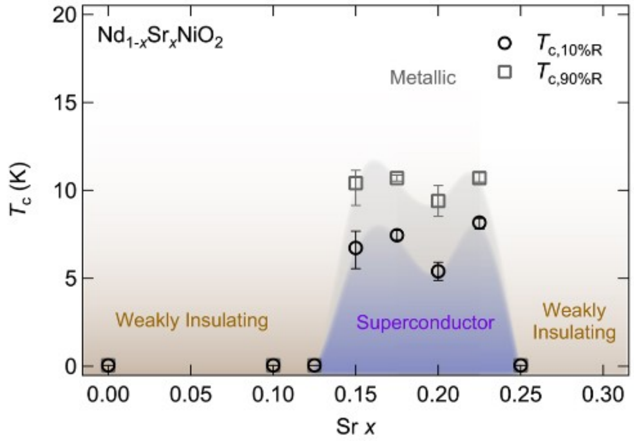
Taillefer et. al., Annual Review of CMP, 1:51-70
PRL 125, 027001 (2020)

Cuprates vs. Nickelates









Taillefer et. al., Annual Review of CMP, 1:51-70
PRL 125, 027001 (2020)

Review & Questions:

➔ Similar oxide planar structure (CuO_2 vs. NiO_2)

➔ Both have 3d9 electronic configuration

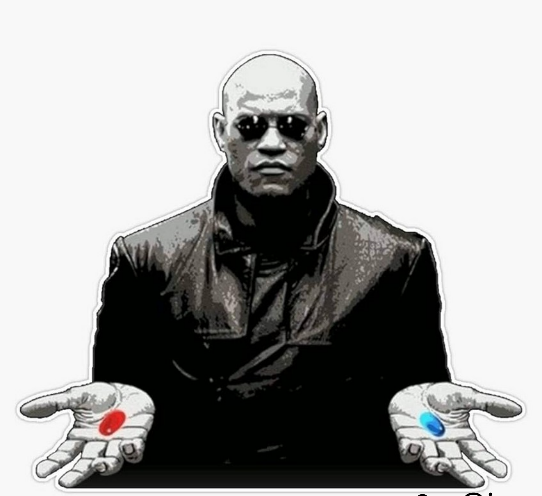
➔ A proxy to understand cuprate superconductivity?

➔ Or, more exotic superconductivity?

➔ Why SC is only seen in thin films?

➔ Role of hole doping

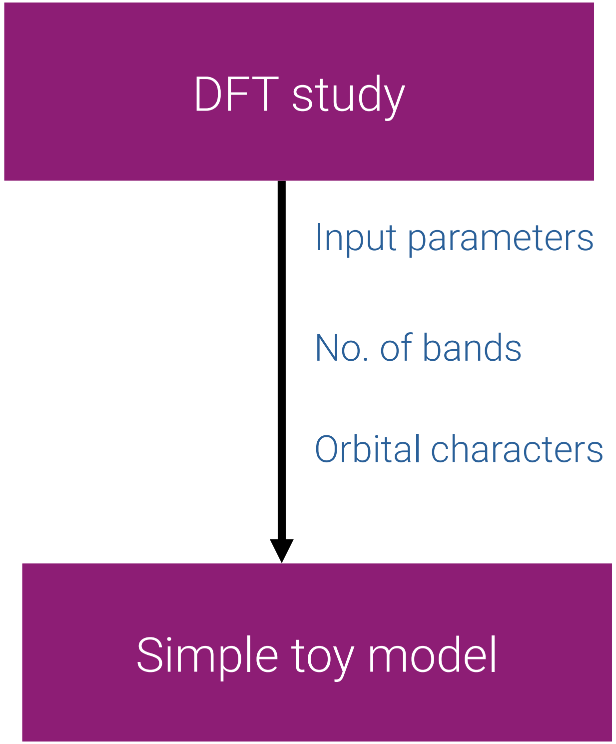
Possible approaches



- Complex models with accurate electronic description
- Reliable results but computationally expensive
- Suitable for small system
- e.g. Density functional theory

- Simpler model with essential physics
- Results depend on input models and parameter; computationally cheap
- Works for larger system
- e.g. Toy model

Density functional theory (DFT)



Density functional theory (DFT)

DFT study

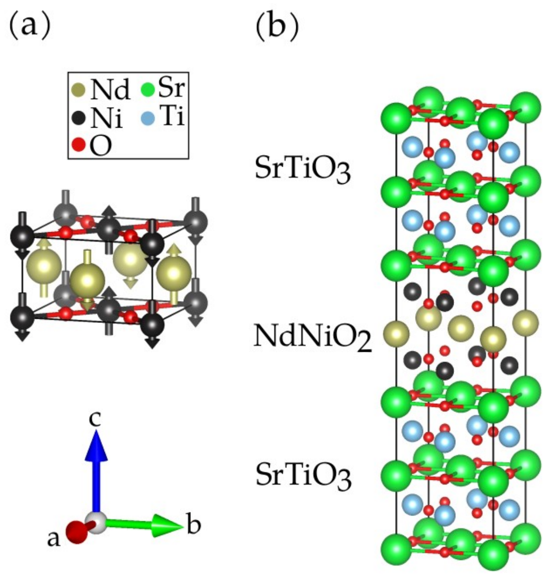
↓ Input parameters

↓ No. of bands

↓ Orbital characters

Simple toy model

- DFT code is implemented by the VASP software
- We take the ground state to be a c-type AFM [see Ptok et al, Condens. Matter 2023, **8**(1), 19]
- Hole-doping is incorporated by taking away electrons
- Optimization > Desnity of states and electronic bands

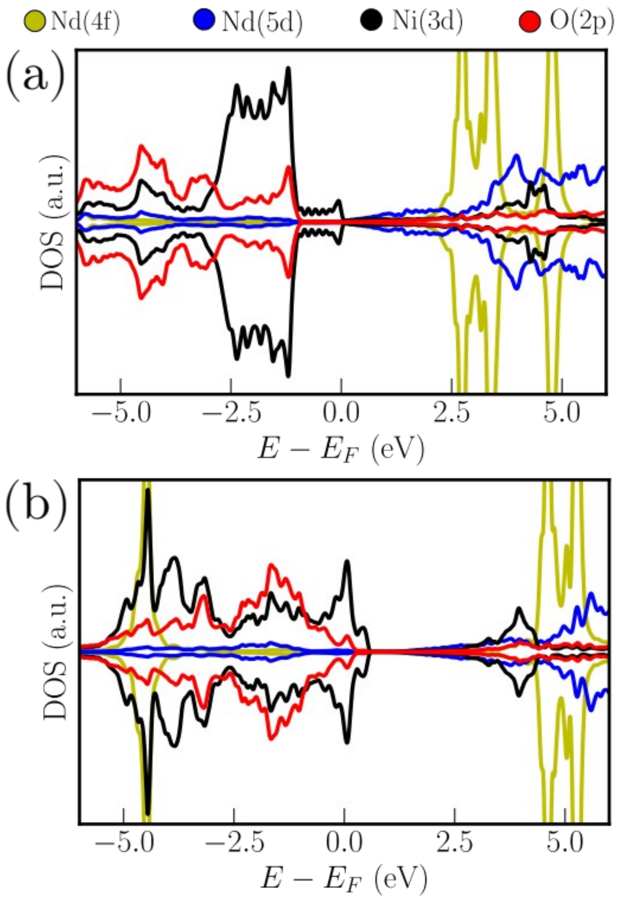


Bulk compound

Thin-film capped by STO

Bulk $NdNiO_2$

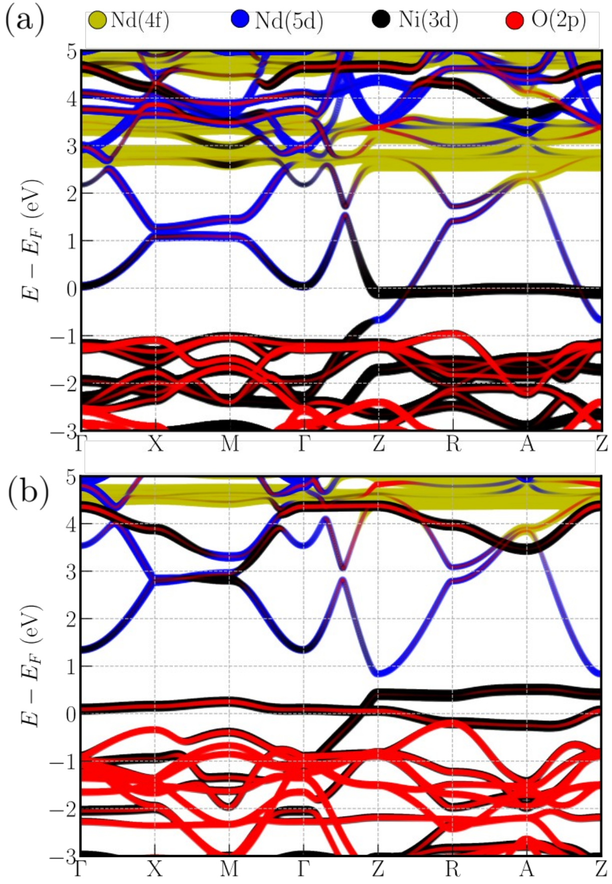
Density of States (DOS)



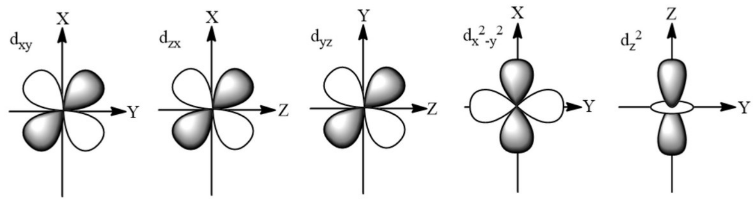
Undoped

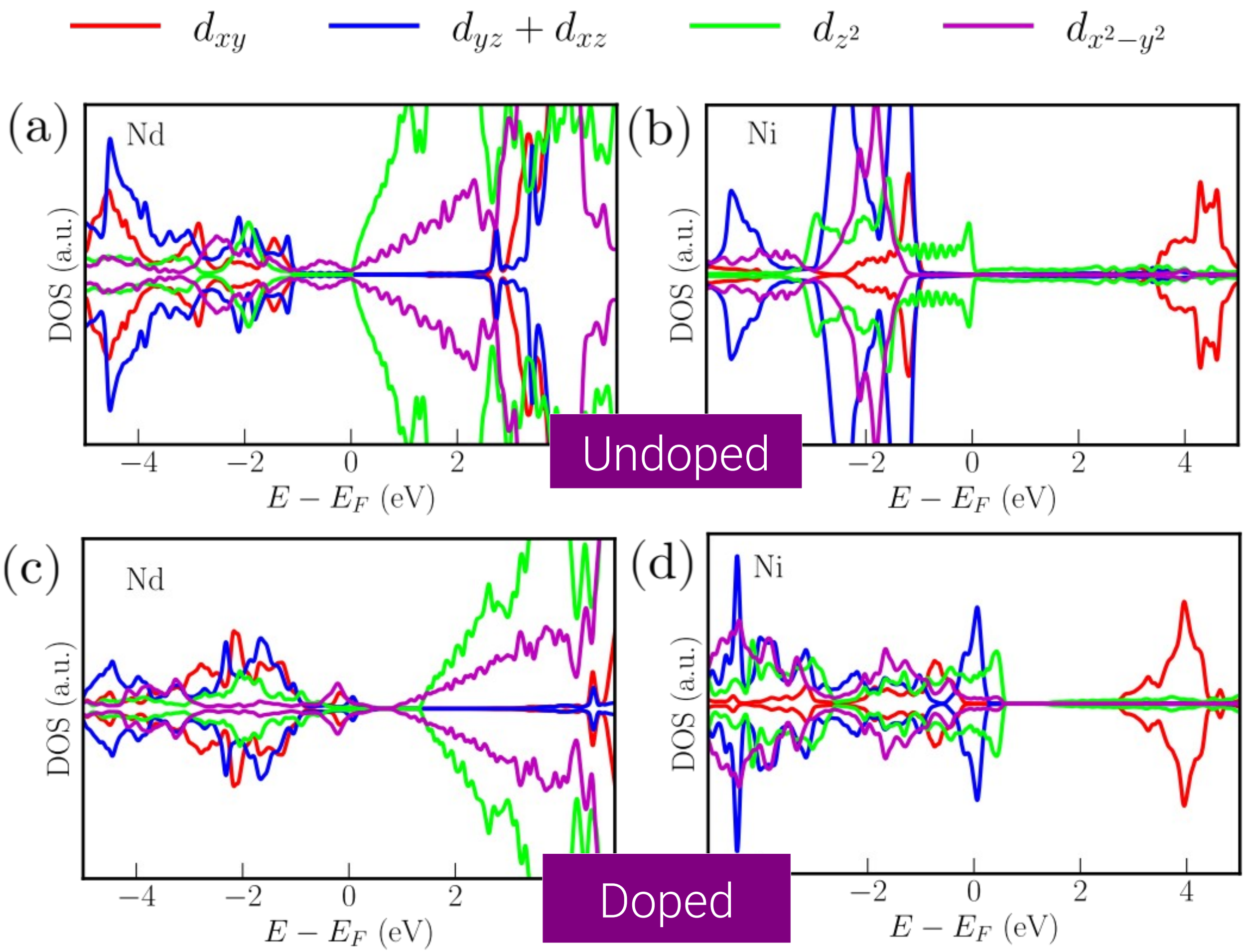
Doped

Electronic bands



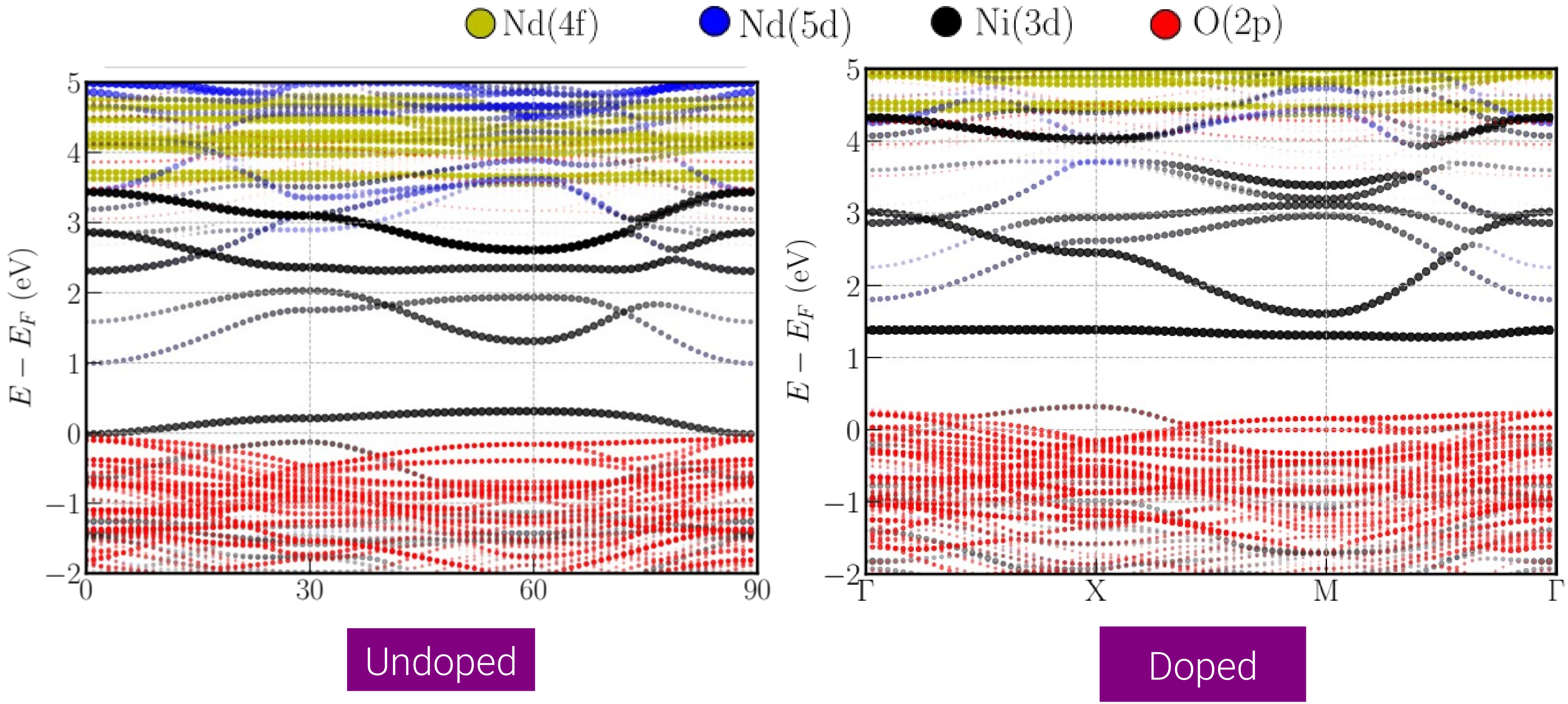
Orbital character





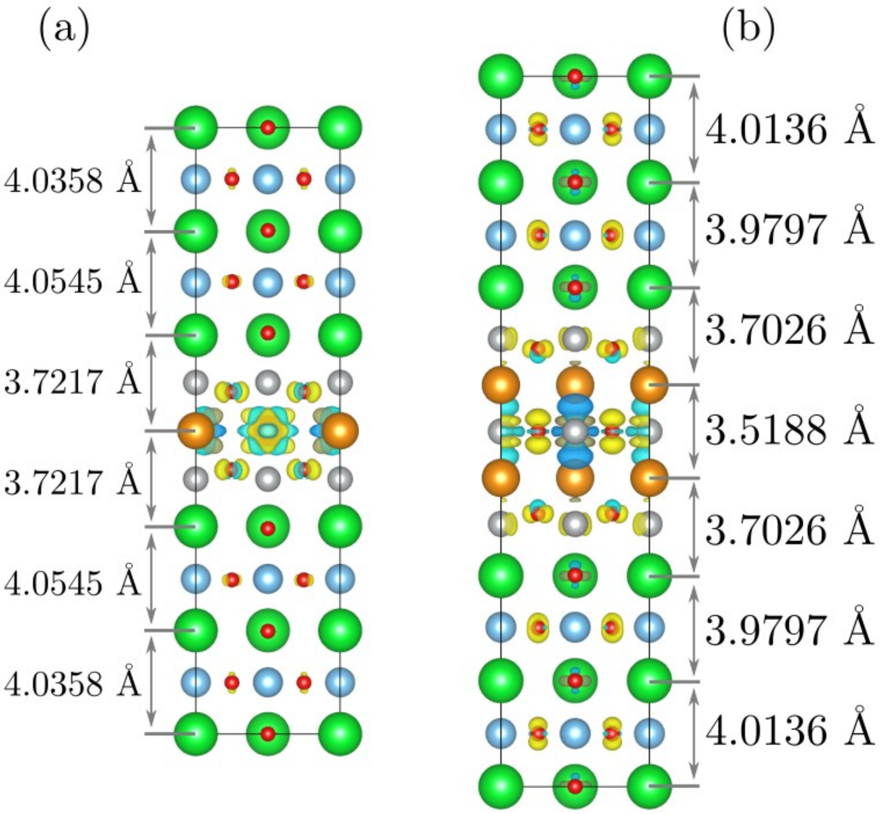
- Ni (3d)-Nd(5d) hybridization
- Parent compound- Ni ($3dz_2$) + Nd ($5dx_2$-y_2) character
- Doped case: Complex interplay b/w several d-orbitals

2 layer thin film



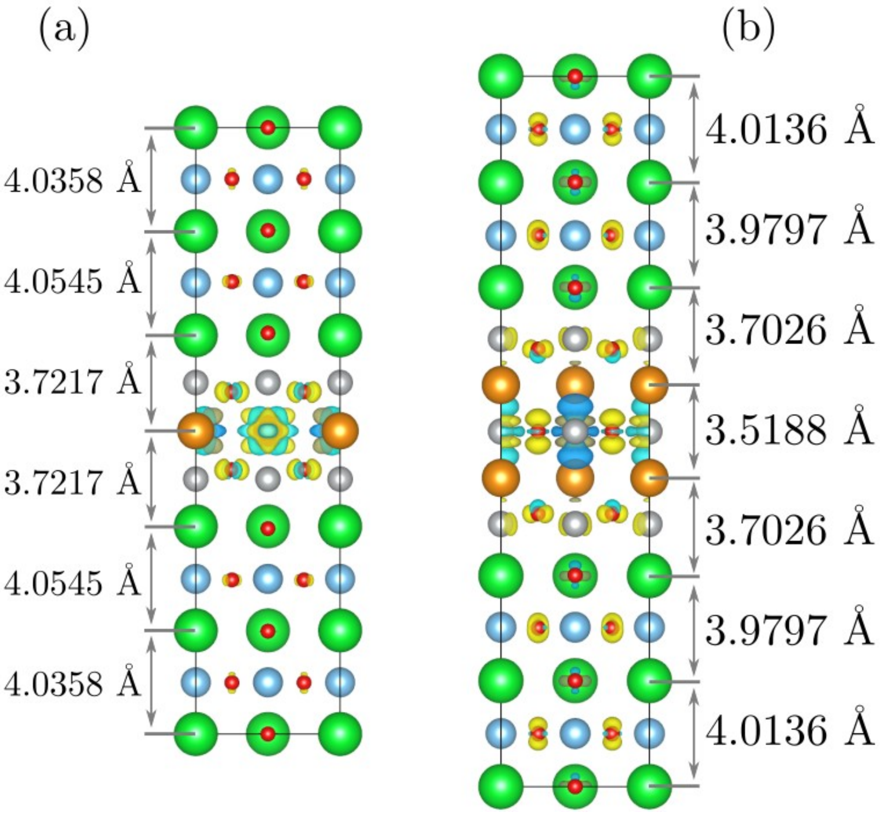
Strong localized Ni 3d bands for the doped case

Charge difference due to hole doping



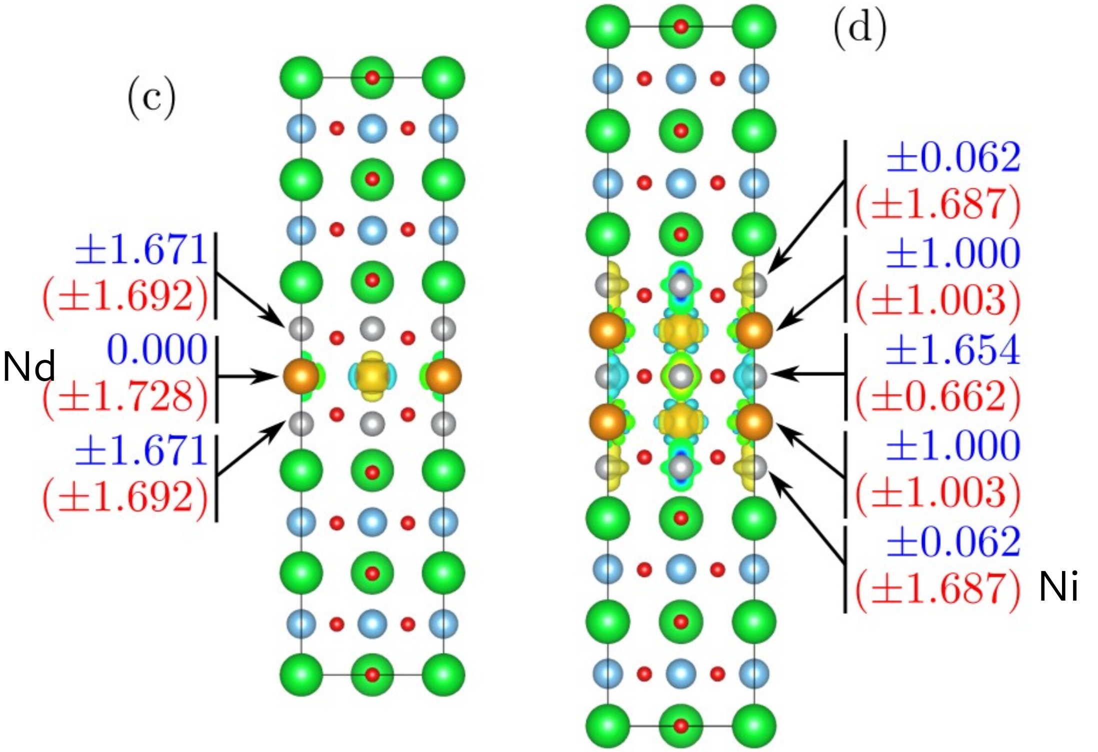
Yellow – e- accumulation
Cyan – e- depletion

Charge difference due to hole doping



Yellow – e- accumulation
Cyan – e- depletion

Magnetic moments for undoped and doped



Blue– undoped
Red –doped

Summary

- Brief intro to high-Tc superconductors, discovery of infinite-layer nickelates
- Contrasting results b/w bulk and thin films compounds
- DFT results suggest strong Ni(3d)-Nd(5d) hybridization, and no effect of Nd(4f) bands
- Orbital character is dominated by Ni(3dz^2), but doped case is complicated
- Rich interplay between interface, strong interaction, and hole doping – more runs are required


Thank
You
Obrigado
Merci
Asante
Arigato
Spasibo
Grazie
Multumesc
Matondo
Dank Je
Maake
Kiitos
Welalin
Juspaxar
Vinaka
Mamana
Nirringrazzjak
Mochchakkeram
Ua Tsaug Rau Koj
Kia Ora
Cam on ban
Chokrane
Salamat
Terma Kasih
Raibh Maith Agat
Matur Nuwun
Dankon