

PHD DAYS PRESENTATION

Probing the crystal and magnetic structure evolution from Perovskite to Brownmillerite In $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_{3-\delta}$

15.02.2024 JCNS-2 FORSCHUNGSZENTRUM JÜLICH

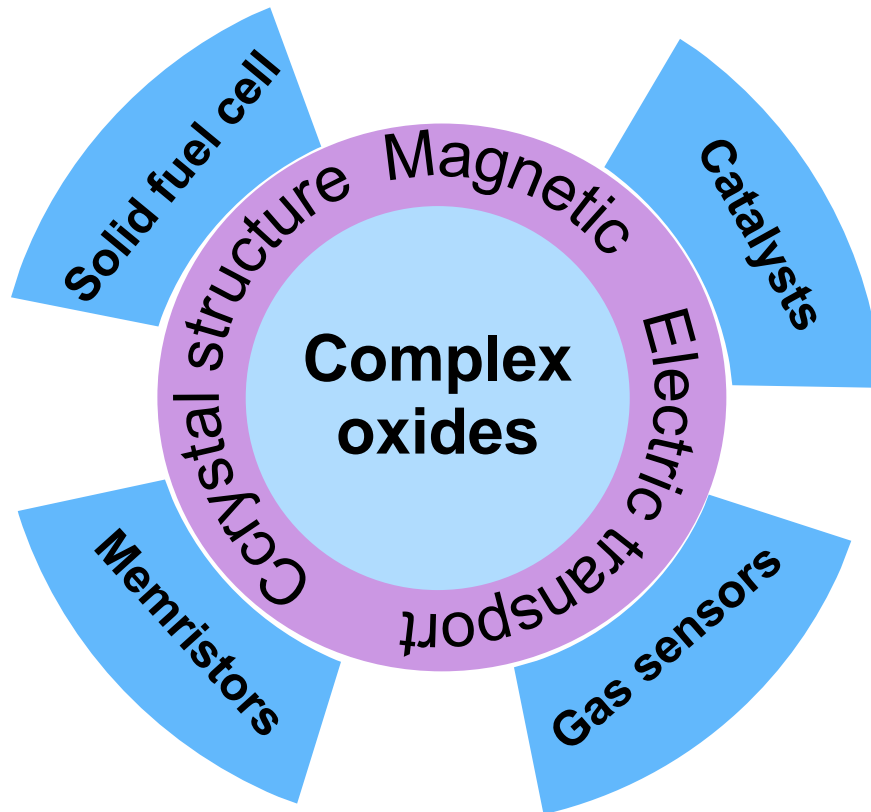
Chenyang Yin, Lei Cao, Suqin He, Felix Gunkel, Denis Sheptyakov, Emmanuel Kentzinger, Sabine Pütter, Mai Hussein, Yifan Xu, Shibabrata Nandi, Asmaa Qdemat, Maria Teresa Fernandez-Diaz, Oleg Petravic

OUTLINE

1. Introduction, motivation and project focus
2. Probing the crystal and magnetic structure evolution from PV to BM at the micro-, meso- and macroscopic length scale
3. Conclusions and outlook

1. INTRODUCTION, MOTIVATION AND PROJECT FOCUS

Complex oxides



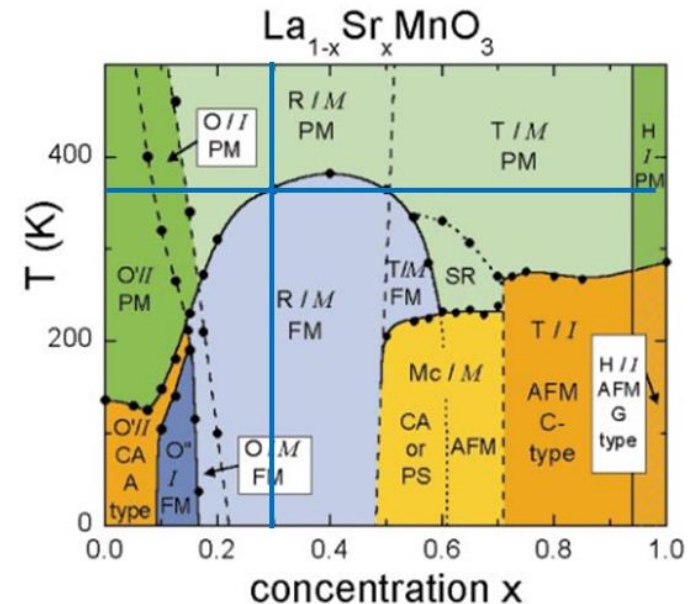
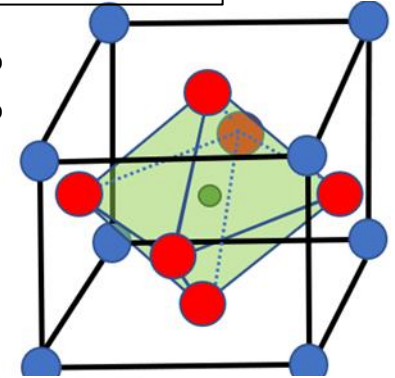
Various applications of complex oxides



A-site ● La^{3+} 70%
 Sr^{2+} 30%

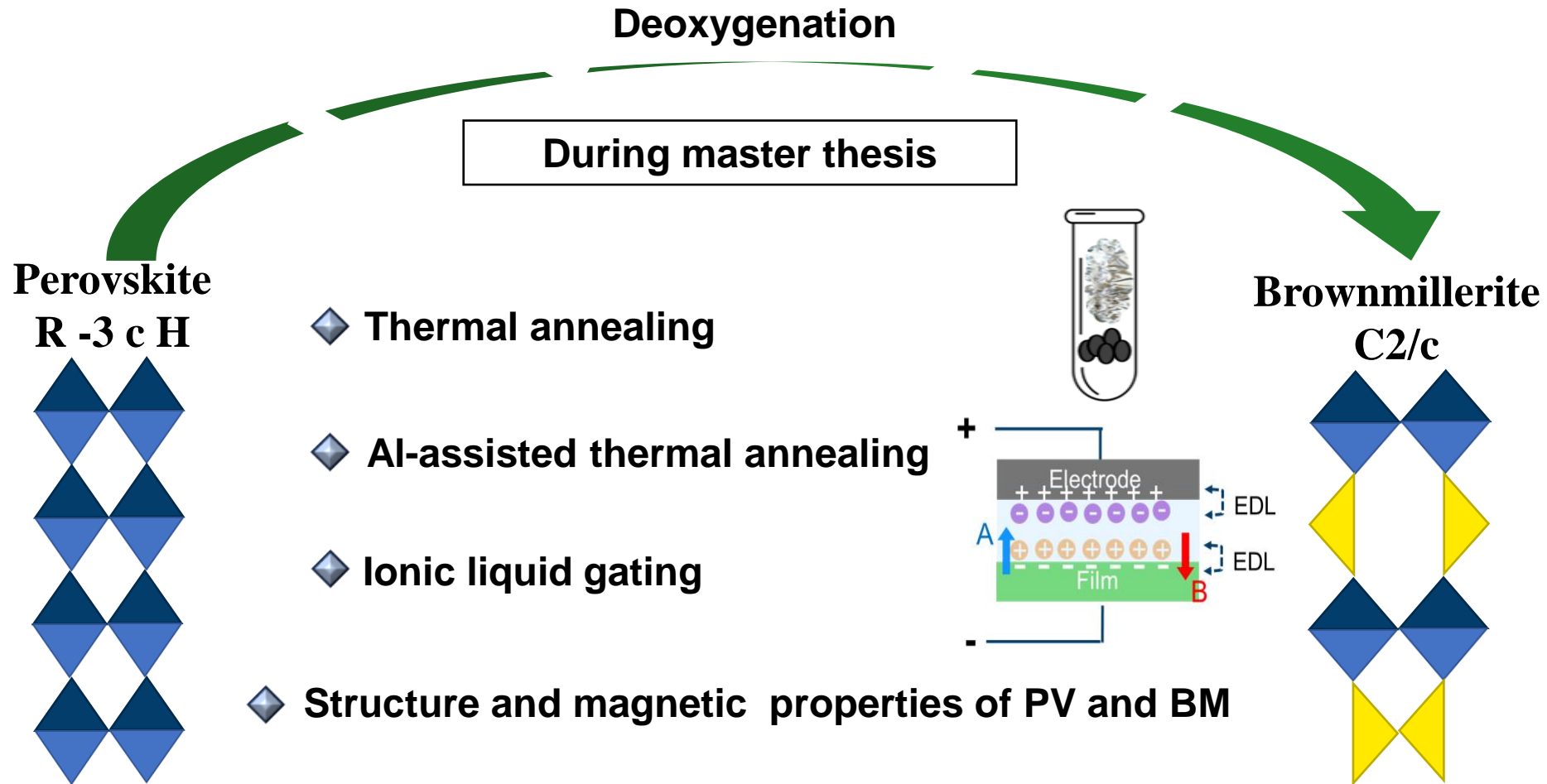
B-site ● Mn^{3+}
 Mn^{4+}

O-site ● O^{2-}

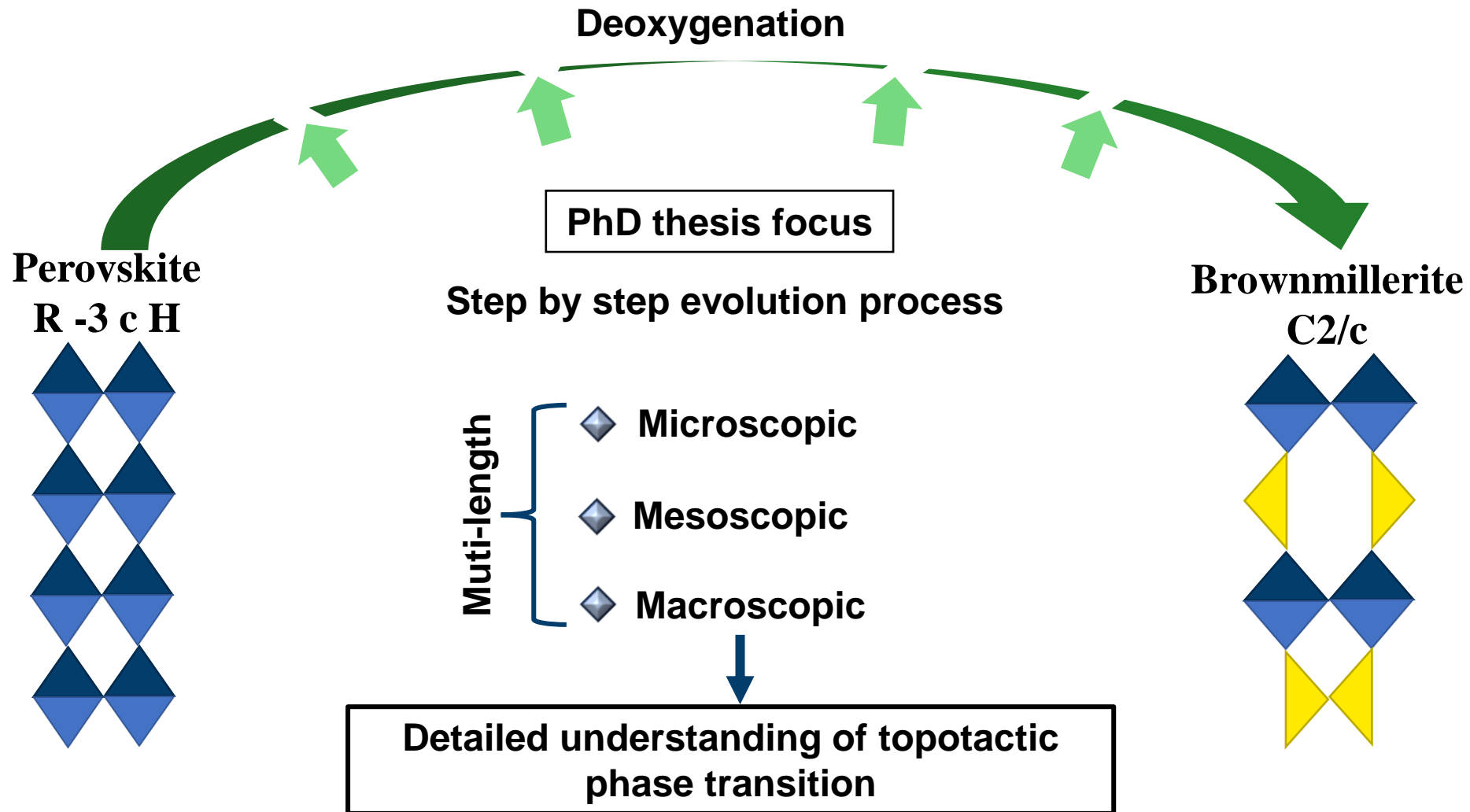


Hemberger, J., et al., *Physical Review B*, 2002.66(9): p. 1-8

1. INTRODUCTION, MOTIVATION AND PROJECT FOCUS

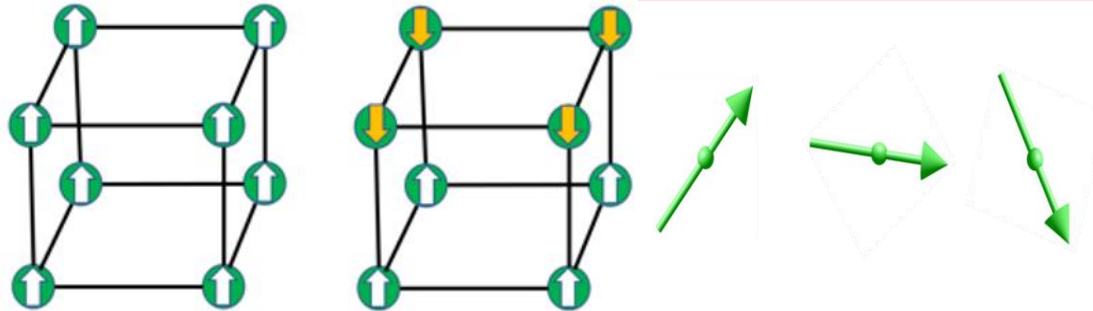


1. INTRODUCTION, MOTIVATION AND PROJECT FOCUS

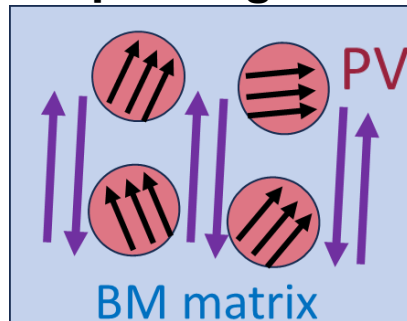


1. INTRODUCTION, MOTIVATION AND PROJECT FOCUS

- ☒ **Microscopic length scale (neutron powder diffraction...)**



- ☐ **Mesoscopic length scale (GISANS,SANS,PEEM...)**



On going project!

- ☒ **Macroscopic length scale (SQUID-magnetometry...)**

FM
Metal

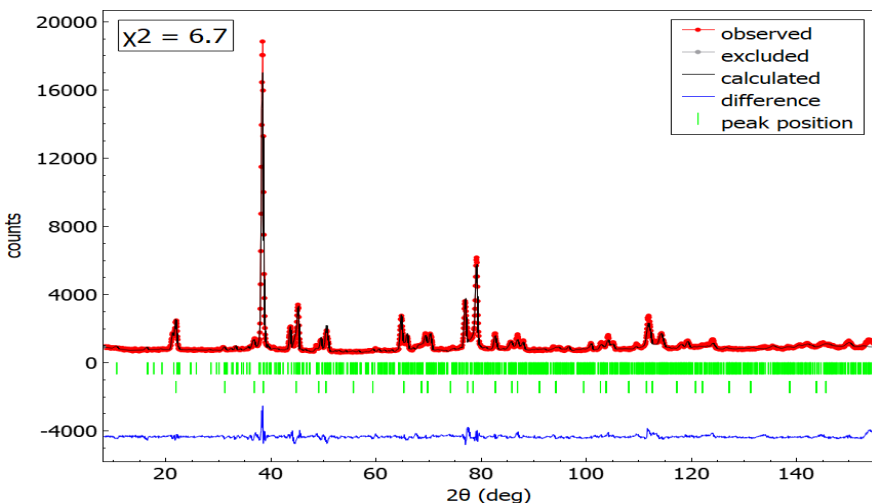


AFM
Insulator

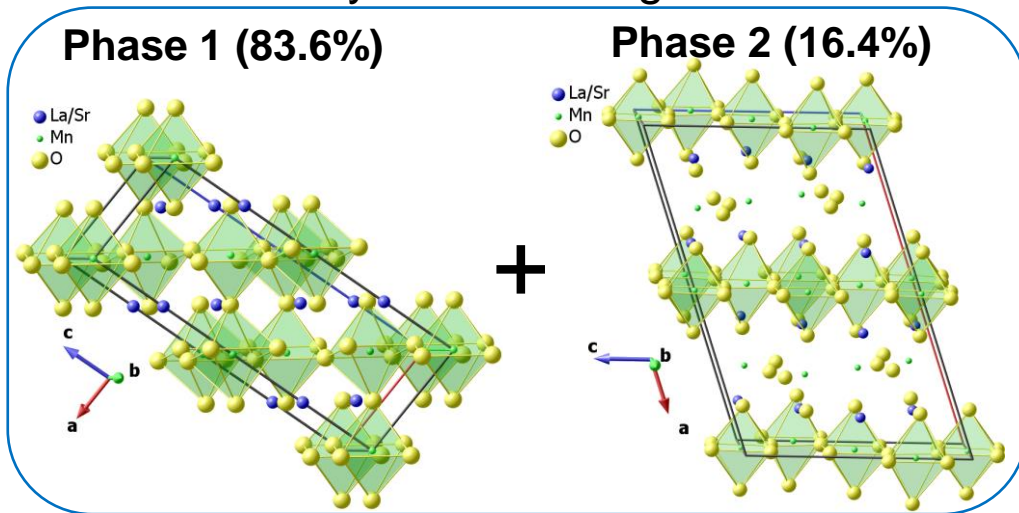
2. THE CRYSTAL AND MAGNETIC STRUCTURE EVOLUTION

LSMO powder, **INTER. 1**, neutron powder diffraction at PSI, HRPT

High T 400K



crystal clustering?



Phase 1: Perovskite (R3-c)167

$$a=5.525\text{\AA} \quad b=5.525\text{\AA} \quad c=13.537\text{\AA}$$

$$\alpha=90^\circ \quad \beta=90^\circ \quad \gamma=120^\circ \quad V=357.9\text{\AA}^3$$

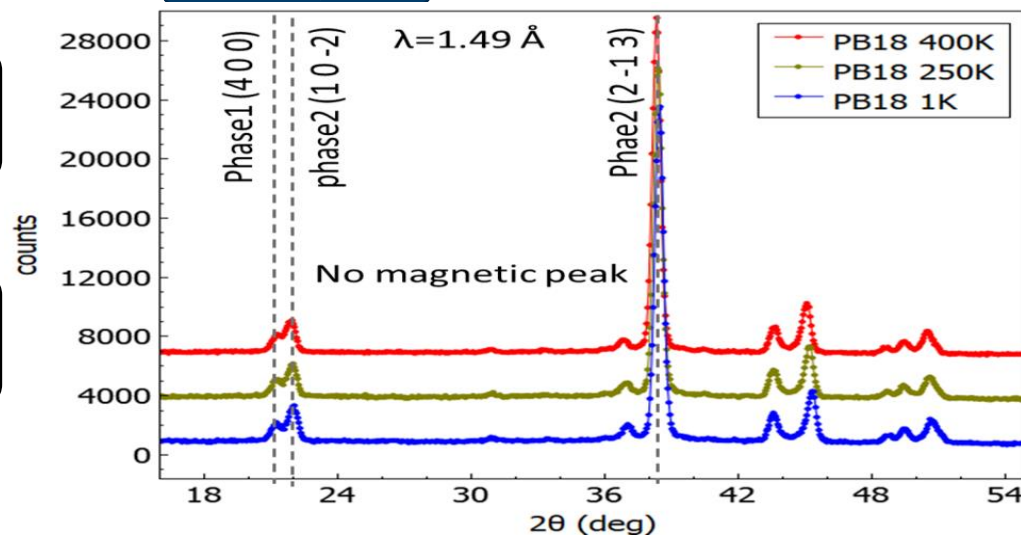
Phase 2: (C2/c) 15

$$a=16.814\text{\AA} \quad b=5.458\text{\AA} \quad c=10.901\text{\AA}$$

$$\alpha=90^\circ \quad \beta=108.707^\circ \quad \gamma=90^\circ \quad V=947.8\text{\AA}^3$$

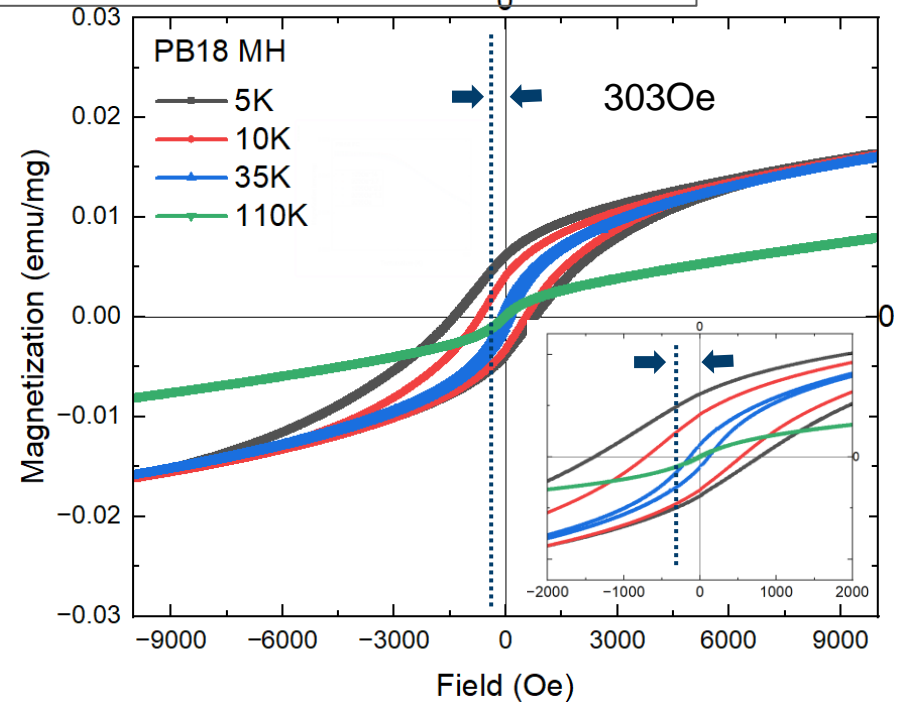
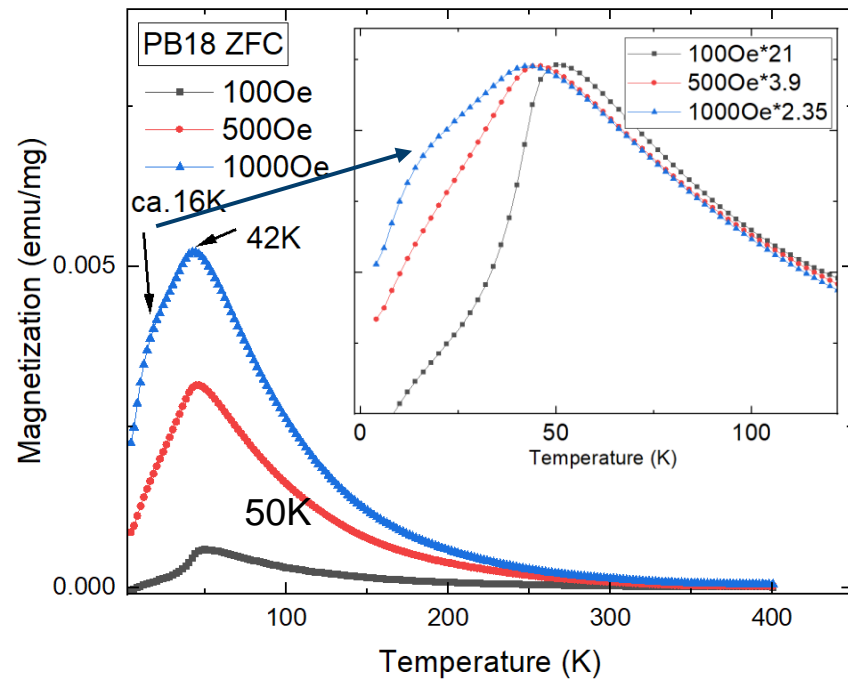
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Low T, 1K



2. THE CRYSTAL AND MAGNETIC STRUCTURE EVOLUTION

LSMO powder, INTER. 1, Vibrating Sample Magnetometer (PPMS-VSM)

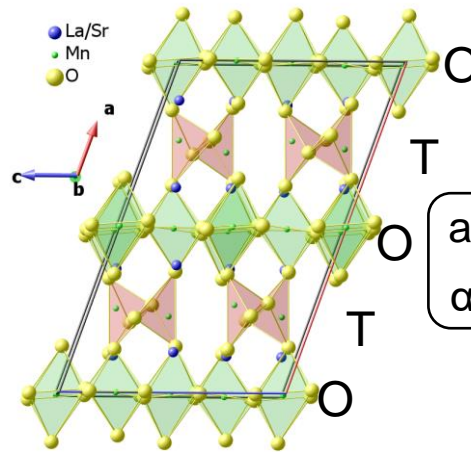
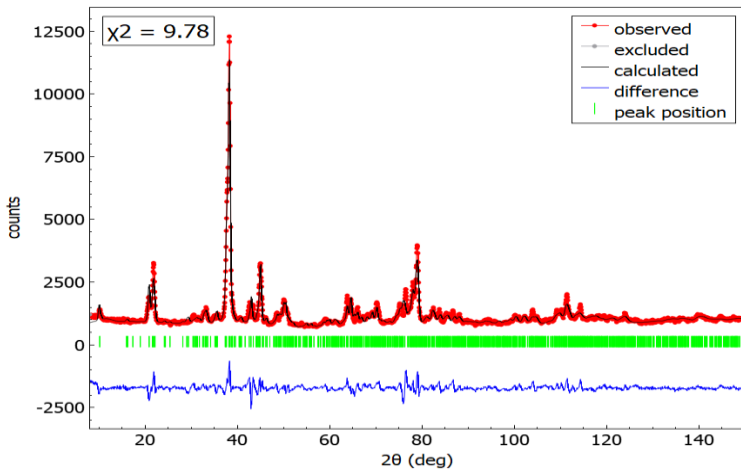


- ◆ Peak at 16 K and at 42 K indicates spin glass state and superparamagnetic state. (need AC-susceptibility)
- ◆ Exchange bias of 303 Oe at 5 K implies the interaction between different magnetic states. e.g. between FM cluster and AFM cluster.

2. THE CRYSTAL AND MAGNETIC STRUCTURE EVOLUTION

LSMO powder, **INTER. 2 (more V_{O})**, neutron powder diffraction at PSI, HRPT

High T 400K

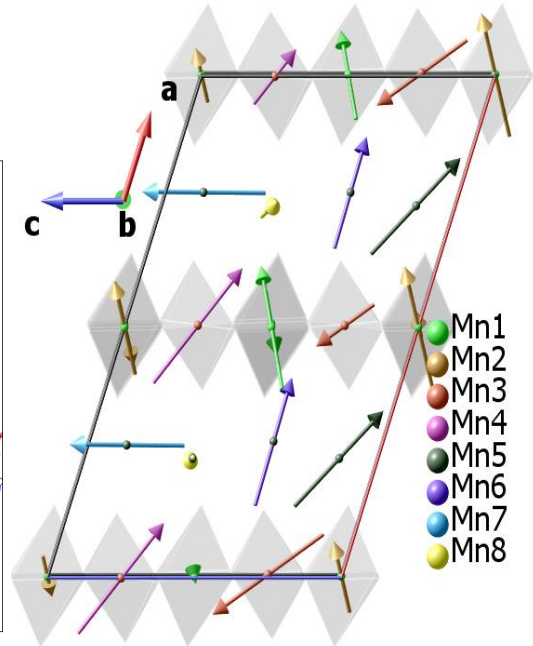
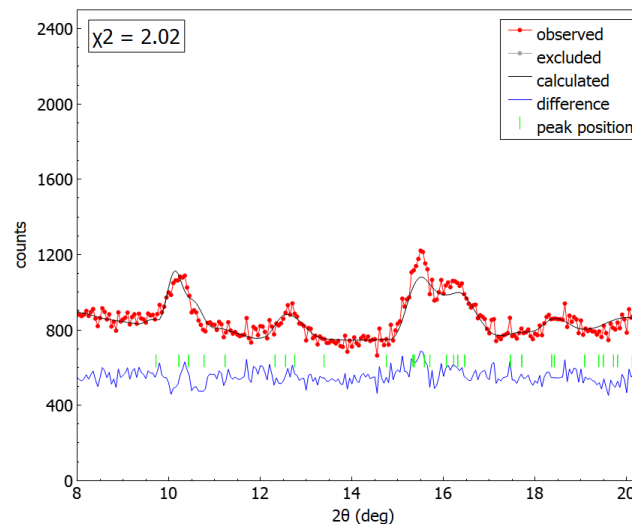
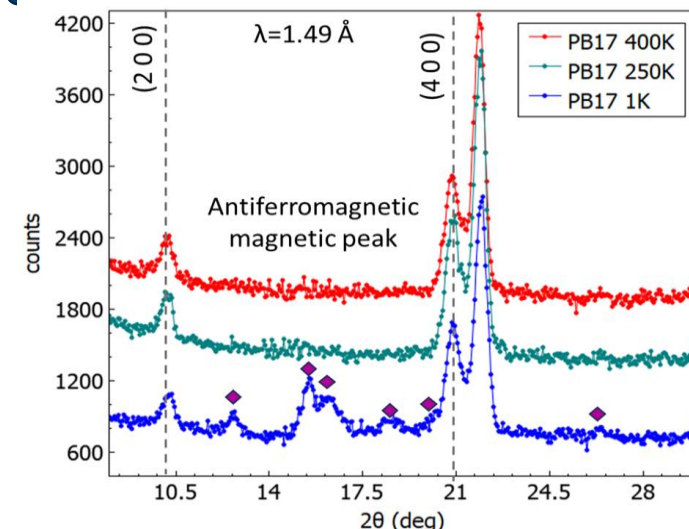


Near-Brownmillerite
(C2/c)₁₅

$$a=17.109\text{\AA} \quad b=5.437\text{\AA} \quad c=10.965\text{\AA}$$
$$\alpha=90^\circ \quad \beta=109.627^\circ \quad \gamma=90^\circ \quad V=961\text{\AA}^3$$

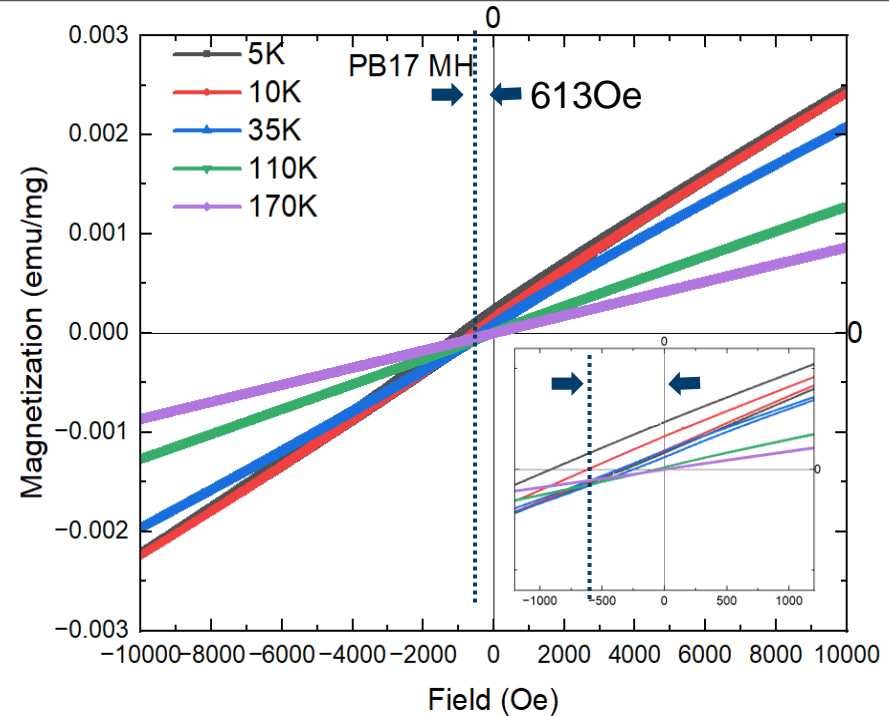
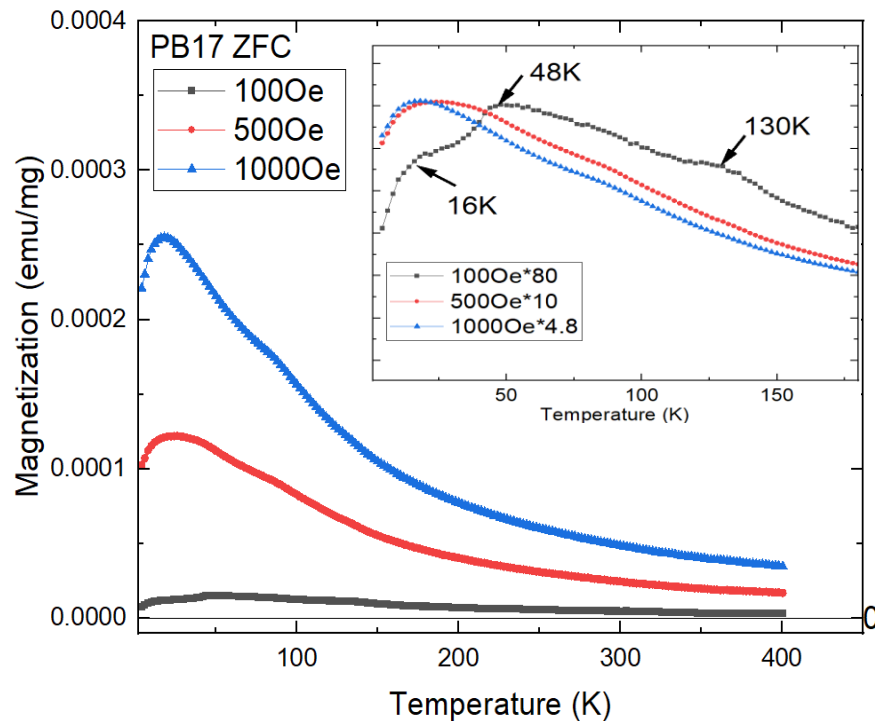
$$Q=(-0.125,0.25,0.15)$$

Low T, 1K



2. THE CRYSTAL AND MAGNETIC STRUCTURE EVOLUTION

LSMO powder, INTER. 2 (more V_{O}), Vibrating Sample Magnetometer (PPMS-VSM)

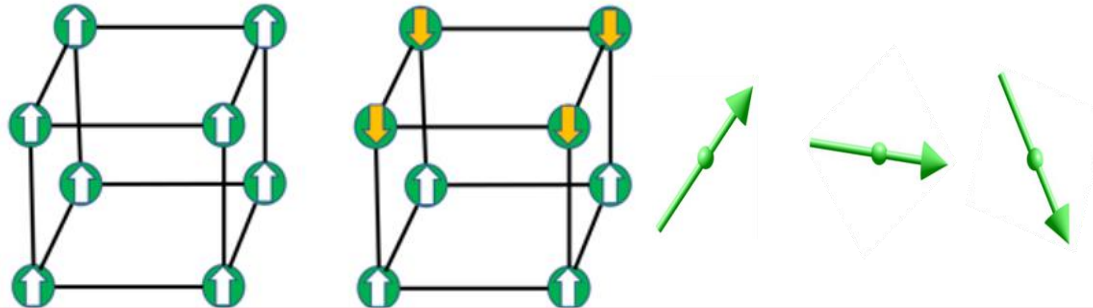


- ◆ 3 Peaks at 16K and at 48K and 130K.
- ◆ Peaks due to AFM at different T? (need neutron thermodiffraction) Or due to AFM+SP+SG? (need AC-susceptibility)
- ◆ Exchange bias of 613Oe of at 5K. ➡ Strong interaction.

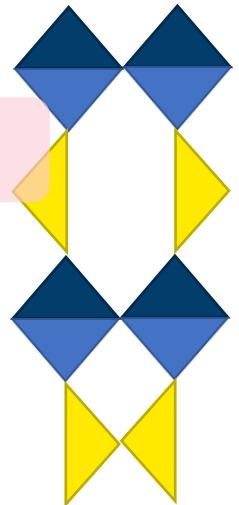
1. INTRODUCTION, MOTIVATION AND PROJECT FOCUS

- ☒ **Microscopic length scale (neutron powder diffraction...)**

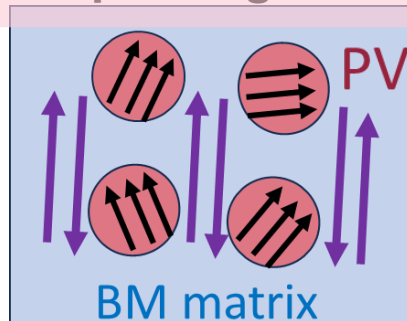
Perovskite
R -3 c H



Brownmillerite
C2/c

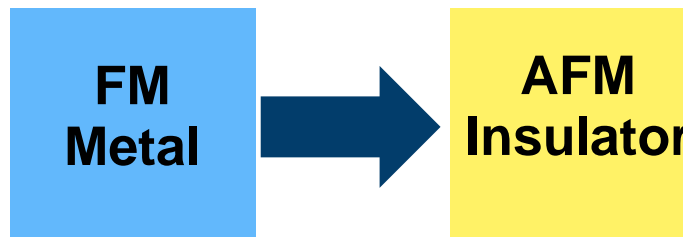


- ☐ **Mesoscopic length scale (GISANS,SANS,PEEM...)**



On going project!

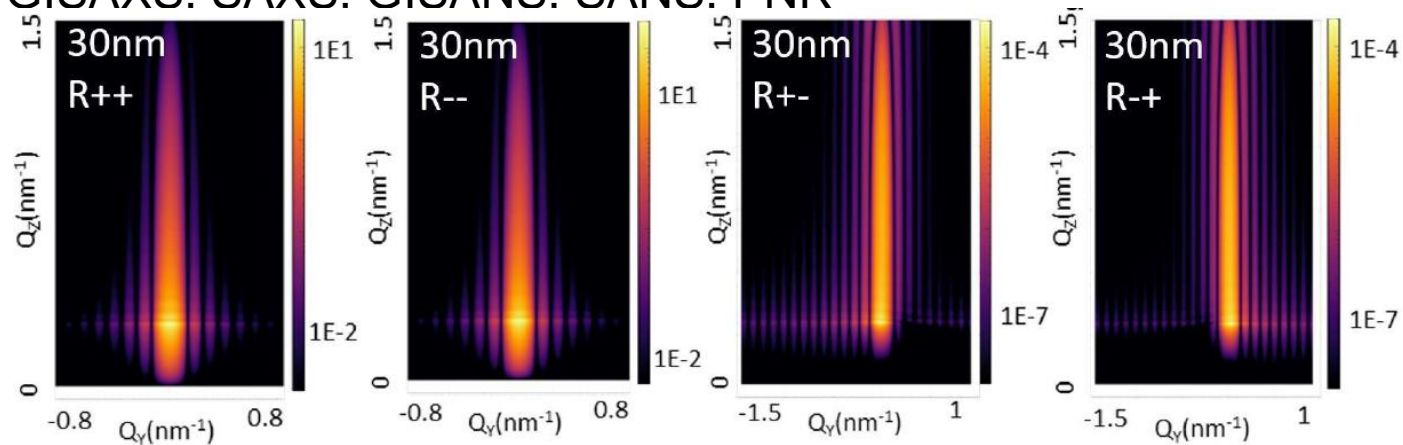
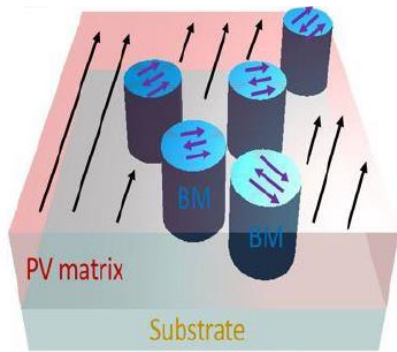
- ☒ **Macroscopic length scale (SQUID-magnetometry...)**



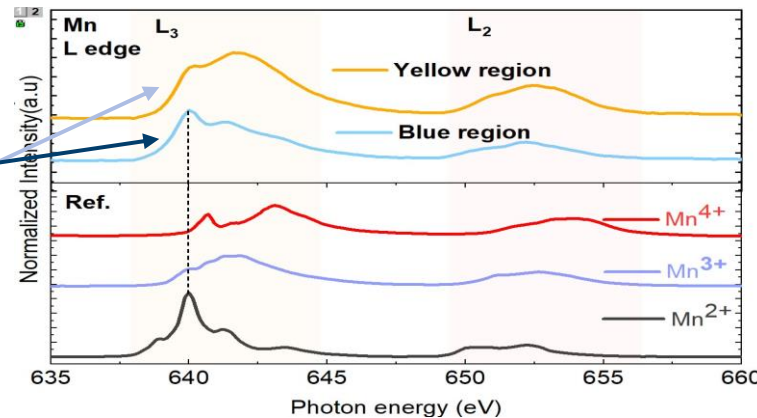
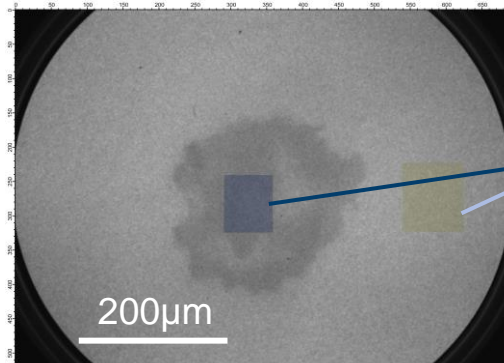
2. THE CRYSTAL AND MAGNETIC STRUCTURE EVOLUTION

Experimental methods for probing mesoscopic information

1. Scattering method: GISAXS. SAXS. GISANS. SANS. PNR



2. Imaging method: PEEM, STXM, STEM

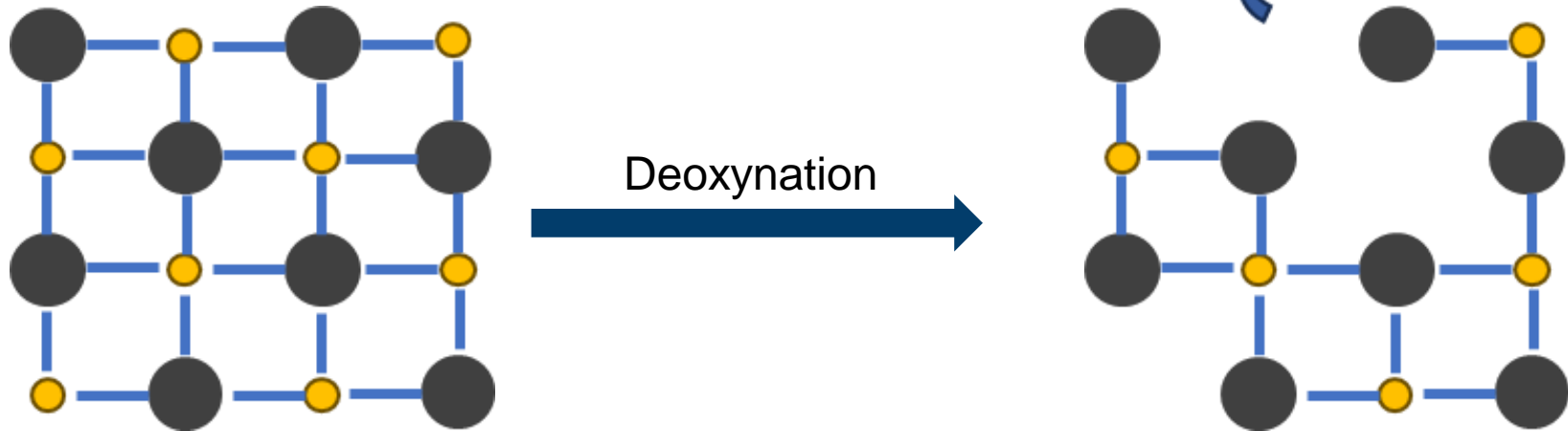


Done by Lei Cao

2. THE CRYSTAL AND MAGNETIC STRUCTURE EVOLUTION

Simulation

Magnetic and electric transport property via simulation?



● Mn

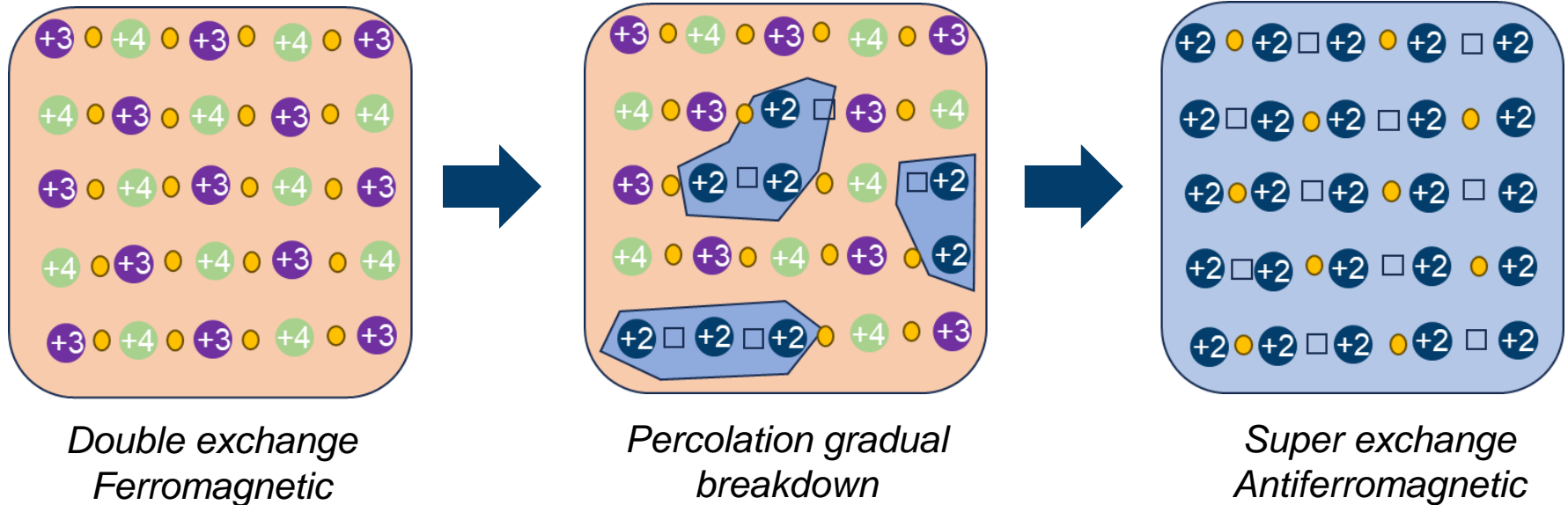
● O

— Magnetic interaction

Percolation theory!

2. THE CRYSTAL AND MAGNETIC STRUCTURE EVOLUTION

Percolation simulation via Monte Carlo method



Plan:

Stage 1: Simple percolation using a 2D matrix (later 3D matrix).  **Current**

Stage 2: Mn oxidation state change induced by oxygen vacancy and the breakdown of double exchange.

Stage 3: Oxygen diffusion.

3. CONCLUSIONS AND OUTLOOK

Conclusions

- The evolution of the crystal and magnetic structure of LSMO powder from PV to BM has been probed in micro- and macroscopic length scales. The results indicate a potential crystal and magnetic clustering process in mesoscopic length scale.

Outlook

- Mesoscopic: the crystal and magnetic clustering process will be continued on the LSMO powder via **SAXS SANS** and on the thin film using **PEEM, STXM, STEM, GISAXS, GISANS, PNR + percolation simulation**.

THANKS FOR YOUR ATTENTION!

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Denis Sheptyakov