INTERNSHIP PROPOSAL

Laboratory name: Institut de minéralogie, de physique des matériaux et de cosmochimie (IMPMC), Sorbonne Université – CNRS – MNHN
CNRS identification code: UMR 7590
Internship director's name: Benjamin Lenz
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Web pages: https://impmc.sorbonne-universite.fr/en/research_teams/quantum-theory-of-matter.html
https://sciences.sorbonne-universite.fr/structures-de-recherche/insp
Internship location: Theory: Sorbonne Université, 4 place Jussieu, 75005 Paris
Experiment: INSP (Sorbonne Université), ESRF synchrotron Grenoble
Thesis possibility after internship: YES
Funding: YES/NO (PhD scholarship from École Doctorale)

Studying doped tetragonal CuO thin films in theory and experiment

Among the 3d transition metal monoxides, CuO is the black sheep of the series. Whereas all its members crystallize in a NaCl-type cubic structure and their Néel temperatures (T_N) follow a monotonically increasing trend, CuO is monoclinic with a rather low T_N, see Fig. 1. Based on this, one might expect a high Néel temperature for CuO with a tetragonal structure (T_N~800–900 K). This would be of interest not only for technological applications, but also from a fundamental standpoint: the antiferromagnetic order would correspond to a large spin-exchange coupling J, which has been linked to superconductivity in the doped copper oxide planes within high-temperature superconducting cuprates.

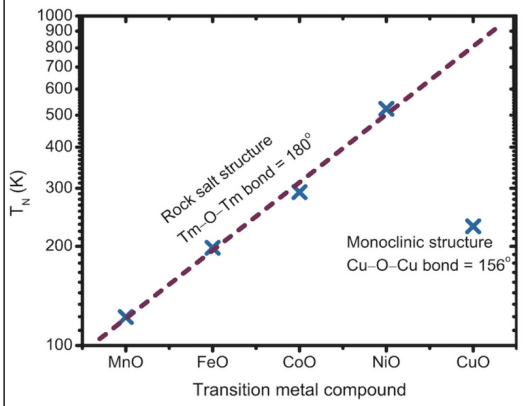


Figure 1: Néel temperatures T_N of different cubic 3d transition metal monoxides TmO, implying for tetragonal CuO T_N~800-900 K [1].

Importantly, CuO in a tetragonal crystal structure (t-CuO) can be stabilized if thin films are grown on a $SrTiO_3$ substrate. Since its first synthesis in 2009 [1], the growth has been optimized, stabilizing t-CuO films of up to ~10 atomic layers. Theoretical methods like density functional theory (DFT) and many-body techniques have allowed to understand most experimental results from techniques like ARPES, RIXS or XMCD [2,3]. Simulations of *hole-doped t-CuO* have suggested the emergence of a superconducting state, which could prove interesting for future experimental studies [2]. Back then, the experimental synthesis of doped t-CuO was unfortunately not possible. This changed recently, when our collaborators succeeded in growing t-CuO layers with chemical substitution of part of the Cu atoms with Co [4]. Also a substitution of some of the O atoms by N is possible, potentially opening new routes to realize the theoretically predicted superconducting state.

But the precise consequences of these substitutions at the structural and electronic level are not clear: Do they lead to structural distortions in t-CuO, to defects, or to a change in its lattice constants? How do these substitutions affect the electronic structure of t-CuO, and how do they alter its magnetic properties?

You will study these questions both theoretically, using DFT+U simulations, and experimentally, using x-ray photoelectron spectroscopy. During your internship you will also be joining a beam time at the ESRF synchrotron to characterize the films structurally, in close collaboration with our colleagues at IPCMS (Strasbourg) and Institut Néel (Grenoble). Also note that this internship can be extended to an overall period of 5-6 months.

References: [1] W. Siemons et al., PRB 79, 195122 (2009) ; [2] B. Bacq-Labreuil et al. PRB 106, 235155 (2022) ; [3] M. Bramberger et al., SciPost Phys. 14, 010 (2023) ; [4] A. Yadav et al., Current Appl. Phys. 90, 40-45 (2026)

Condensed Matter Physics: YES Soft Matter and Biological Physics: NO
Quantum Physics: MAYBE Theoretical Physics: MAYBE
Physics of Energy and Climate Dynamics: NO