NÉEL INSTITUTE Grenoble

Topic for Master 2 internship – Academic year 2024-2025

High T_c superconductivity in layered $Ln_{n+1}Ni_nO_{3n+1}$ nickelates

General Scope:

The search of high T_c superconductivity in other analogous materials than cuprates has started more than 35 years. For Ni, the discovery of unconventional superconductivity in thin film of hole-doped infinite-layer nickelate $Nd_{1-x}Sr_xNiO_2$ (with square planar coordinated Ni^+ in d^9 configuration for x = 0) below T_c = 15 K (for x~0.2) by the group of H.Y. Hwang (Stanford) mid-2019 has suddenly intensified the research in this field. So far, no superconducting bulk nickelates were discovered until the recent report of superconductivity near 80 K in $La_3Ni_2O_{7-\delta}$ (La-327) under high pressure (HP) by M. Wang et al. (China). On the contrary of previous nickelates this bilayer compound shows a mixed valency state $Ni^{2.5+}$ (i.e. d^7/d^8) and several theoretical scenarios have been proposed to understand the related high T_c superconductivity mechanism but the question is not yet resolved. Like cuprates, La-327 shows a $3d_{x^2-y^2}$-based Fermi surface but also an additional pocket involving $3d_{z^2}$ orbitals which is potentially crucial. In fact, superconductivity occurs just above a structural phase transition at P* ~ 10-14 GPa, where the Ni-O_{apical}-Ni angle, closely related to oxygen 2p/nickel $3d_{z^2}$ orbitals hybridization, changes from 168° to 180° [Fig. 1]. In addition, superconductivity has also been detected in the trilayer $La_4Ni_3O_{10-\delta}$ nickelate, with a lower maximal T_c, around 30 K at 69 GPa and also with a similar phase transition around 15 GPa involving apical oxygens by Y. Zhu et al.

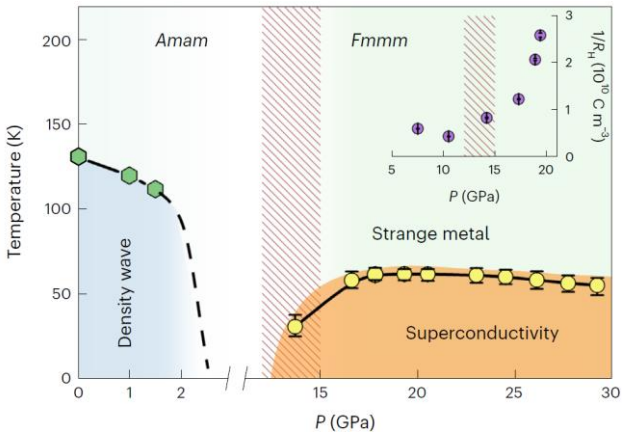

Fig. 1 P,T phase diagram of La-327 [Sun et al., Nature 621, 493 (2023) ; Zhang et al. Nat. Phys. 20, 1269 (2024)].

Research topic and facilities available:

In fact, P* is closely related to hydrostaticity conditions and/or oxygen vacancies content (δ). In early studies a transition from *Amam* to *Fmmm* space groups (both orthorhombic) was reported. Since 2019, at Néel Institute we are working on related infinite-layer Ni oxides. In MRS group, we have also synthesized several $Ln_{n+1}Ni_nO_{3n+1}$ compounds, in particular the n = 2 and 3 members. Thanks to x-ray diffraction (XRD) experiments under high high pressure (HP) conducted on different synchrotrons x-ray sources (ESRF, SOLEIL and Elettra) we have shown that in good hydrostatic conditions (with helium as pressure medium) P* is ~ 6.5-8 GPa for La-327 and is related to an orthorhombic – tetragonal transition (towards *I4/mmm*). During this internship we will complement these results by studying other properties, like the magnetic ones, via the development of magnetization/HP. We will also focus our studies on samples with lower defects levels ($La_2PrNi_2O_{7-\delta}$). A last objective will be to try to stabilize superconductivity in these layered nickelates at (nearly) ambient pressure thanks to adequate chemical substitution and/or the use of new synthesis techniques. Possibly another XRD/HP study at SOLEIL will be planned during the internship and resistivity or Raman spectroscopy measurements under (/HP) measurements in collaboration with MagSup team.

Possible collaboration and networking: We have currently a joint research ANR project on nickelates with CRISMAT in Caen and several laboratories in Parisian region.

Possible extension as a PhD: this internship will be extended into a PhD where potential superconductivity in palladates will also be explored. Funding may be obtained via the Physics Graduate School of Grenoble.

Required skills: A good background in material science and condensed matter physics is required.

Starting date: Spring 2025

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