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# Interface-Induced Modifications on the Atomic and Electronic Structures of $La_3Ni_2O_7$

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The recent discovery of superconductivity at approximately 80 K in the Ruddlesden–Popper (RP) phase bilayer nickelate $La_3Ni_2O_7$ under high-pressure conditions has led to extensive follow-on studies [1-5]. The RP nickelate phases are characterized by a layered perovskite structure, with $n$ $NiO_2$ layers interspersed between rock salt LaO layers. The occurrence of superconductivity in bilayer $La_3Ni_2O_7$ is necessitated by both the extreme pressures involved and the desire to understand the intricate interactions between the different layers. In $La_3Ni_2O_7$, the Ni ions possess an average $3d^{7.5}$ configuration, indicating partially occupied $d_{x2-y2}$ and $d_{z2}$ orbitals. This unique electronic structure, coupled with strong electron correlations that give rise to superconducting pairing with both intralayer and interlayer characteristics [2–4], suggests a novel mechanism of superconductivity in this material.

One of the main challenges in the synthesis of high-quality single crystals of $La_3Ni_2O_7$ arises from its narrow synthesis window [6]. This limitation inevitably leads to the formation of monolayer ($n = 1$, $La_2NiO_4$) and trilayer ($n = 3$, $La_4Ni_3O_{10}$) phases [7], which complicate the properties and characterization of the material. These adjacent phases can potentially alter the crystal and electronic structures, but their precise influence remains poorly understood and difficult to predict. In this study, we investigate how the interfaces—specifically the interactions between the monolayer/bilayer and trilayer/bilayer interfaces—impact the structure and electronic behavior of the bilayer $La_3Ni_2O_7$ phase.

To elucidate the local structural and electronic modifications resulting from interface interactions, aberration-corrected scanning transmission electron microscopy (STEM) coupled with monochromated electron energy loss spectroscopy (EELS) was employed. To comprehensively analyze both heavy and light atoms, multiple imaging techniques were used simultaneously, including high-angle annular dark-field (HAADF) and annular bright-field (ABF) STEM (Fig. 1). Atomic-scale EELS enabled layer-by-layer investigation of local electronic structure variations along the interfaces (Fig. 2). Complementary density functional theory (DFT) simulations support the observed modifications in the atomic and electronic structures. Based on these multifaceted results, we argue that interfacial interactions should not be overlooked, and a deeper understanding of these effects is crucial to explaining the superconductivity observed in bilayer nickelates [8, 9].

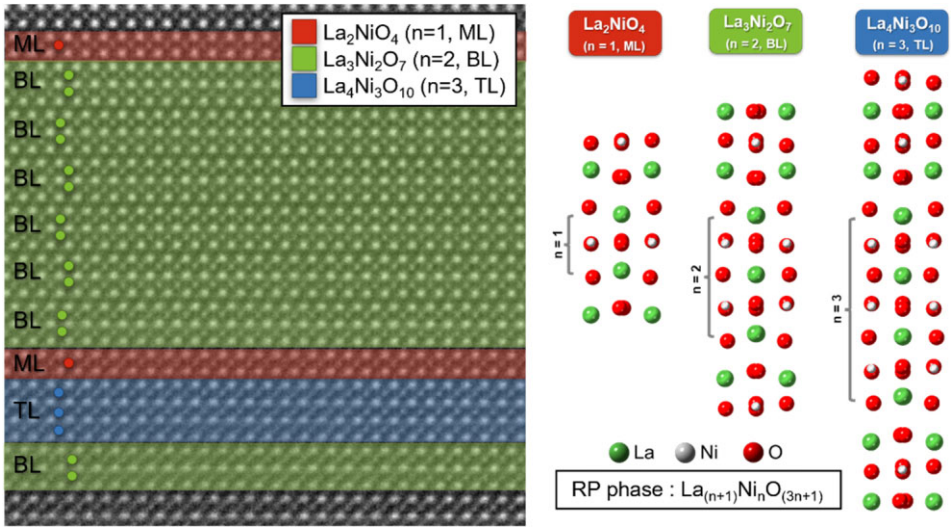


**Figure 1.** HAADF-STEM image of $La_3Ni_2O_7$ (n = 2, bilayer), exhibiting a mixture of $La_2NiO_4$ (n = 1, monolayer) and $La_4Ni_3O_{10}$ (n = 3, trilayer). The background color varies according to the n values. On the right, schematic representations of the atomic structures of RP nickelate phases, $La_{n+1}Ni_nO_{3n+1}$, are presented.

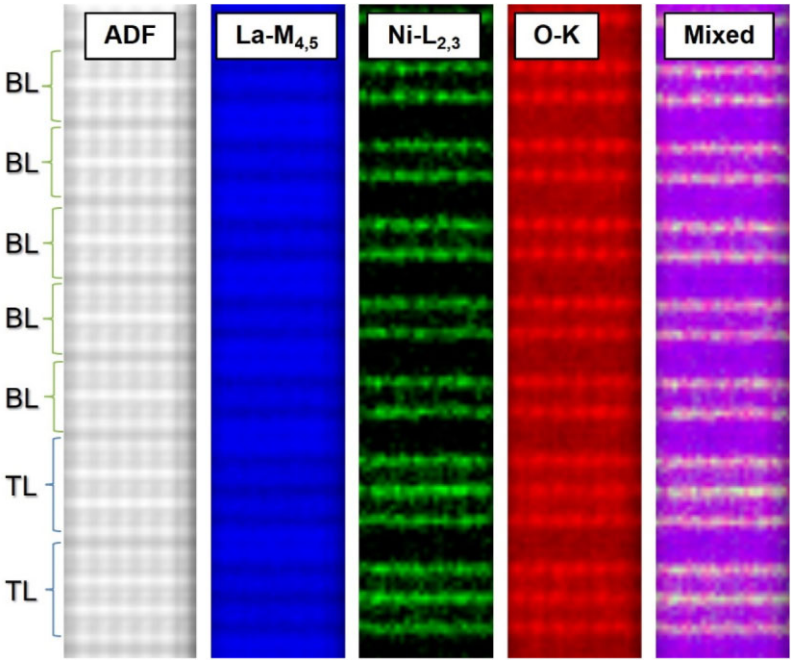


**Figure 2.** Atomic-resolution STEM-EELS maps of the La $M_{4,5}$ edge, Ni $L_{2,3}$ edge, and O K edge, highlighting elemental distributions in bilayer and trilayer nickelates.

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