# Possible *s*±-Wave Superconductivity in Heavily Hole-Doped Infinite-Layer Nickelates: A Theoretical Study Based on First Principles

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Recently, a high-temperature superconductor $La_3Ni_2O_7$ has attracted significant attention due to its transition temperature ($T_c$), which is comparable to those of cuprates [1]. Although the pairing symmetry remains a subject of ongoing debate, the bilayer Hubbard model is widely considered to capture the essential physics of $La_3Ni_2O_7$. Theoretical studies suggest that *s*±wave superconductivity with a high $T_c$ can emerge in the bilayer model when the interlayer hopping integral $t_\perp$ is sufficiently large [2]. This bilayer model can be mapped onto a two-orbital model [3], where the bonding and antibonding bands correspond to orbitals with lower and higher energies, respectively, and the energy offset $\Delta E$ between the two orbitals corresponds to $t_\perp$. Here, we refer to such two-orbital systems as the Orbital-Space Bilayer Model (OSBM). Recently, we proposed possible manifestations of the OSBM in a Ba-based cuprate [4] and nickel oxychlorides [5]. In the latter materials, we demonstrated that multi-orbital models involving more than two orbitals can exhibit s±-wave superconductivity driven by the same mechanism as in the OSBM.

In this presentation, we propose heavily hole-doped infinite-layer nickelate thin films as promising candidates for realizing the OSBM [6]. We have constructed a five-orbital tight-binding model, incorporating all five $3d$ orbitals, constructed via Wannierization based on the crystal structure energetically optimized through first principles calculation. The effects of epitaxial strain from the substrate are explicitly taken into account by fixing the in-plane lattice constants to match those of the substrate. Under compressive strain, the crystal-field splitting between the $d_{x^2-y^2}$ orbital and the other orbitals is enhanced, leading to a larger $T_c$. By applying the fluctuation exchange approximation to this five-orbital model, we show a substantial enhancement in the eigenvalue λ of the Eliashberg equation in the hole-doping range of $x = 0.6 - 0.8$. This result indicates that *s*±-wave superconductivity is strengthened in this heavily hole-doped region.

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