Possible Superconductivity in Hole-doped $La_3Ni_2O_6$: A Theoretical Study Based on the Orbital-Space Bilayer Model

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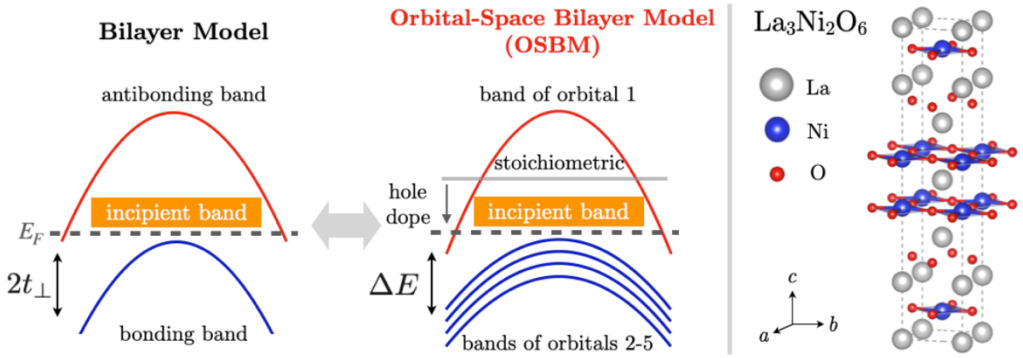
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Bilayer models have theoretically been proposed as a route to superconducting transition temperatures higher than those of conventional cuprates [1]. A notable example is the recently discovered bilayer nickelate superconductor $La_3Ni_2O_7$ [2]. Meanwhile, an equivalence between bilayer systems and two-orbital systems has been demonstrated through a basis transformation in Ref.[3], where the bonding-antibonding splitting in the former corresponds to the orbital level offset. ΔE in the latter. We have previously studied the possibility of superconductivity in multiorbital systems and found that superconductivity is optimized, similarly to the bilayer models, when ΔE is large and in the presence of "incipient bands," whose band edge lies near the Fermi level [4-6]. We refer to such multiorbital systems as the Orbital-Space Bilayer Model (OSBM).

Although no OSBM-based superconductors have yet been experimentally reported, we focus on $La_3Ni_2O_6$, whose synthesis has already been established, as a candidate material [7]. $La_3Ni_2O_6$has a NiO_2 square-planar structure that produces a large orbital level offset ΔE, favorable for OSBM-based superconductivity. Although superconductivity has not been reported in $La_3Ni_2O_6$, we theoretically investigate the possibility of realizing superconductivity through hole doping, which brings the system closer to the incipient-band regime [8].

By constructing a tight-binding model based on first-principles calculations, a large ΔE between the Ni $d_{x^2-y^2}$ and the other 3d orbitals is obtained. Furthermore, our fluctuation exchange (FLEX) approximation calculations indicate the emergence of s±-wave superconductivity driven by interorbital interactions in an incipient-band situation, where the superconducting gap function changes its sign between the $d_{x^2-y^2}$ and other d orbital bands. We will also discuss structural stability under pressure and elemental substitution, as well as possible structural phase transitions.



(Left) Correspondence between the bilayer model and orbital-space bilayer model. In both cases, superconductivity is optimized in the incipient-band situation. (Right) Crystal structure of $La_3Ni_2O_6$.

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