Theoretical Analysis of Electron Correlation Effects on High-Pressure Superconductivity in Infinite-Layer Nickelates Using an Effective Model

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The infinite-layer nickelates RNiO$_2$ (R=La, Nd, Pr) were proposed based on their electronic-structure similarity to cuprate superconductors. In these materials, the quasi-two-dimensional NiO$_2$ conducting planes are formed by transition-metal Ni^{1+} ions, and the Ni $d_{x^2-y^2}$ orbital dominates the electronic states near the Fermi level (E_F). The superconducting transition temperature (T_c) of these systems at ambient pressure is approximately 10–20 K, which is lower than that of cuprate superconductors (T_c = 40–135 K). However, recent experiments on freestanding $Nd_{0.85}Sr_{0.15}NiO_2$ membranes released from their growth substrates, which enable high-pressure measurements beyond the limitations of substrate-bound thin films, have shown that the onset superconducting transition temperature (T_c^{onset}) increases monotonically with hydrostatic pressure and reaches 70–80 K at pressures up to about 90 GPa [1].

The ratio of the Coulomb interaction to the hopping integral, U/t, measures electron-correlation strength in strongly correlated systems, where an optimal value exists to maximize T_c. In nickelate superconductors, it has been suggested that the U/t value of the $d_{x^2-y^2}$ orbital lies on the strongly correlated side of this optimum, and that excessive electron correlations may suppress superconductivity [2]. The purpose of this study is to theoretically explain the pressure-induced enhancement of T_c and to clarify its underlying mechanism [3].

We have performed first-principles calculations to optimize the crystal structure under pressure. Then phonon calculations confirmed that the tetragonal $P4/mmm$ structure remains dynamically stable up to 90 GPa. Subsequently, a seven-orbital tight-binding model reproducing the electronic structure near E_F was constructed as an effective low-energy model using Wannier functions. Electron-electron interactions calculated from first principles were incorporated into this model. By applying the fluctuation-exchange (FLEX) approximation to this model [4], the eigenvalue λ of the linearized Eliashberg equation, a measure of superconducting stability, was evaluated. We assumed d-wave pairing symmetry throughout the analysis.

In our seven-orbital model, the derived Coulomb interaction U remains nearly unchanged under pressure, whereas the nearest-neighbor hopping integral t of the $d_{x^2-y^2}$ orbital increases substantially, leading to a significant reduction of U/t. Additional calculations using models in which the parameter were hypothetically varied indicate that the pressure-induced variations in hopping parameters are the primary origin of the pressure dependence of λ. Applied pressure also induces self-doping through an enlargement of rare-earth-derived electron pockets, which tends to weaken d-wave pairing. Despite this adverse effect, the reduction of U/t dominates, resulting in enhanced superconducting pairing. The monotonic increase of λ is consistent with the experimentally observed increase in T_c, indicating that the enhancement of T_c under high pressure is attributed to the mitigation of excessive electron correlations.

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