Supplmental material : Theoretical study on the possibility of high T_c $s\pm$-wave superconductivity in the heavily hole-doped infinite layer nickelates

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PHONON DISPERSION OF $LA_{1-x}SR_xNIO_2$

In Fig. S1, we present the calculated phonon dispersion of $La_{1-x}Sr_xNiO_2$ for all the cases (combination of the Sr content and the substrate) considered in the present study. As seen from these results, imaginary frequencies do not appear in any of the cases, indicating that the $P4/mmm$ symmetry of the original $LaNiO_2$ is dynamically stable.

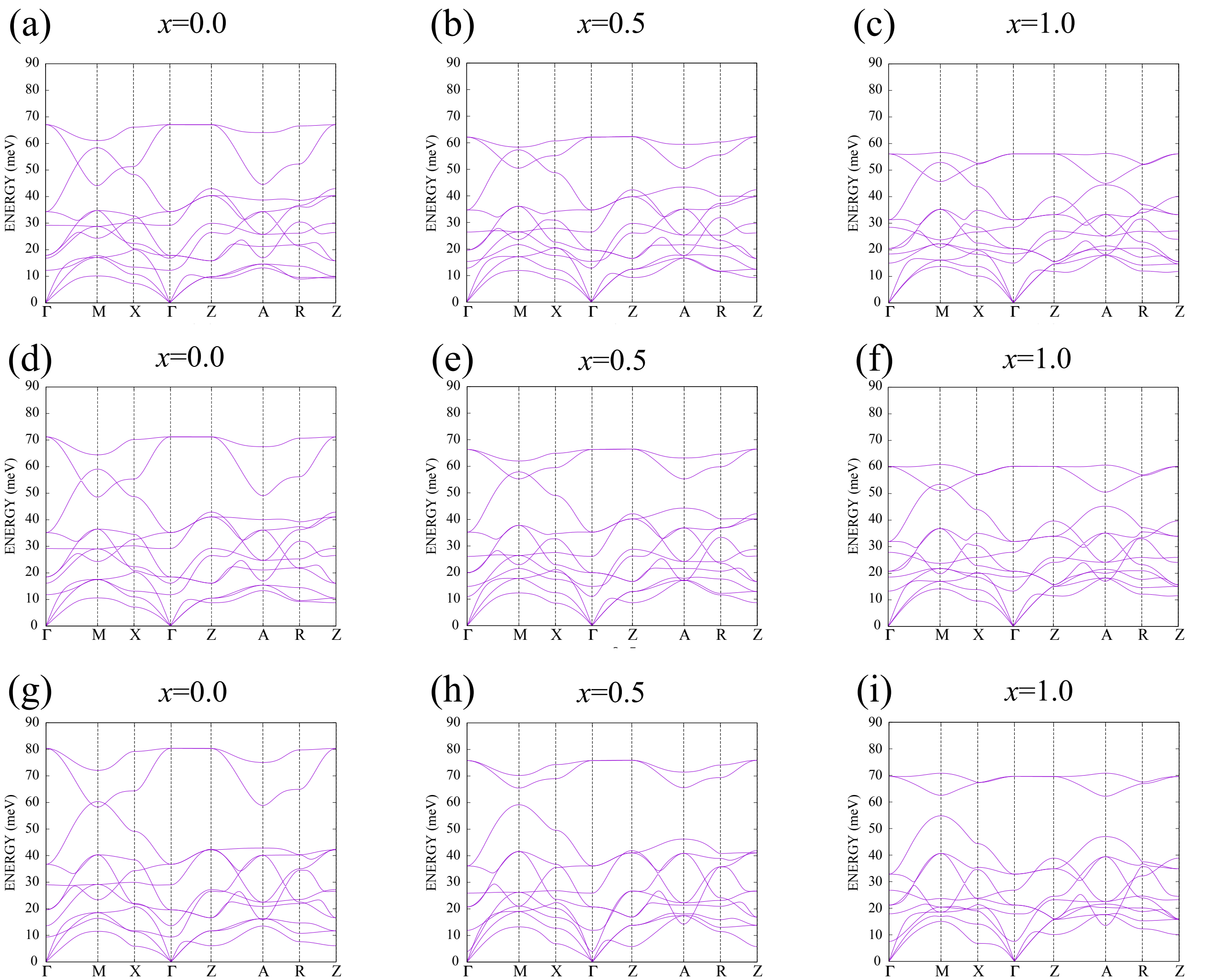

FIG. S1. The phonon dispersion of $La_{1-x}Sr_xNiO_2$ with the in-plane lattice constant fixed to that of $SrTiO_3$ ((a)-(c)), LSAT ((d)-(f)), or $LaAlO_3$ ((g)-(i)) substrates. The Sr content is $x = 0$ ((a),(d),(g)), $x = 0.5$ ((b),(e),(h)), or $x = 1$ ((c),(f),(i)).

ELECTRONIC BAND DISPERSION OF $LA_{1-x}SR_xNIO_2$

In Fig. S2, we present the calculated electronic band dispersion of $La_{1-x}Sr_xNiO_2$. The Ni-d bands other than the $d_{x^2-y^2}$ band become incipient at x ∼0.5–0.7 for $SrTiO_3$ and LSAT substrates and x ∼0.7 for $LaAlO_3$ substrate.

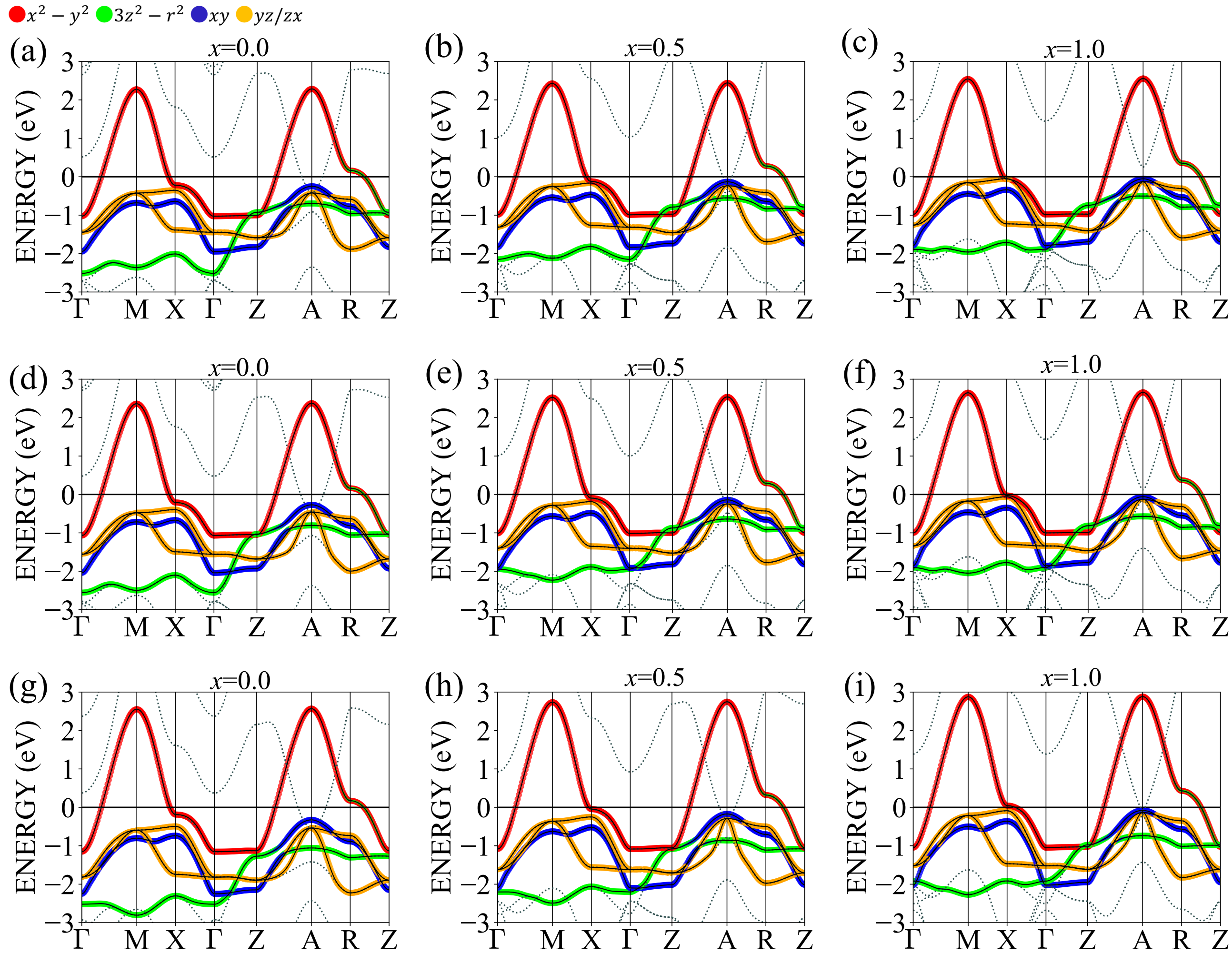

FIG. S2. The electronic band dispersion of $La_{1-x}Sr_xNiO_2$ with the in-plane lattice constant fixed to that of $SrTiO_3$ ((a)-(c)), LSAT ((d)-(f)), or $LaAlO_3$ ((g)-(i)) substrates. The Sr content is $x = 0.3$ ((a),(d),(g)), $x = 0.5$ ((b),(e),(h)), or $x = 0.7$ ((c),(f),(i)). The strength of the Wannier orbital characters are shown with the thickness of the color coded line.

LATTICE MISMATCH BETWEEN $LA_{1-x}SR_xNIO_2$ THIN FILM AND SUBSTRATES

In Fig. S3(a), we present the lattice constants of a and c of $La_{1-x}AE_xNiO_2$(AE =Ba, Sr) against the substitution ratio x. The lattice constant a becomes smaller because of the smaller ionic radius of Sr ion than that of La. In contrast, the constant c in the AE=Ba case becomes larger, probably affected by the ionic radius of Ba.

In Fig. S3(b), we present the mismatch of the lattice constants between thin film and substrates against the ratio x. It can be seen that the mismatch is below 2% for the $SrTiO_3$ and LSAT cases throughout the range of x. Even for the case of $LaAlO_3$, for the higher substation ratio, the mismatch is below 2%.

EFFECTS OF GGA+U METHOD

In Fig. S4, we show the band dispersion calculated by GGA+U method. Compared to Fig. S2, the splittings bands between the $d_{x^2-y^2}$ orbital and the other orbitals are larger. This is because that the energy of the filled (not filled) orbitals is pushed up (down) from the Fermi level in the GGA+U calculations.

In Fig. S5, we plot the eigenvalues λ against the ratio x for comparison with the GGA result. The change of λ is probably caused by that of the band splitting. Namely, in the GGA+U case, d-bands become father from the Fermi level, so that larger amount of holes are required to make these bands incipient. This is the reason why higher doped

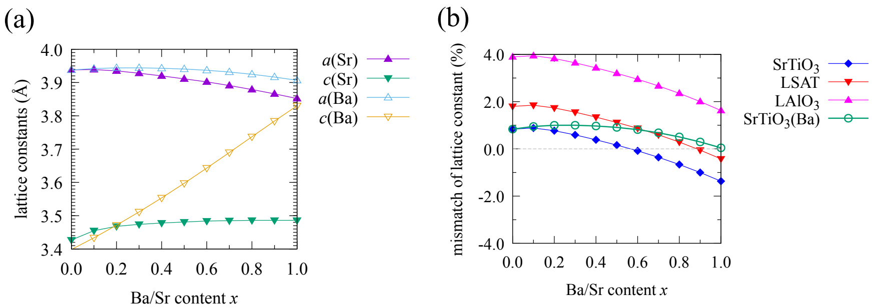

FIG. S3. (a) The lattice constants of a and c of $La_{1-x}AE_xNiO_2$(AE =Ba, Sr) against the ratio x and (b) the mismatch of the lattice constants between the thin film and substrates. Here, the legends indicate the three substrates (with the lattice constants 3.905, 3.868, 3.790 Å for $SrTiO_3$, LSAT, $LaAlO_3$, respectively). In panel (b), the AE=Ba case is indicated by open symbols, while the other cases (AE=Sr) are indicated by filled symbols.

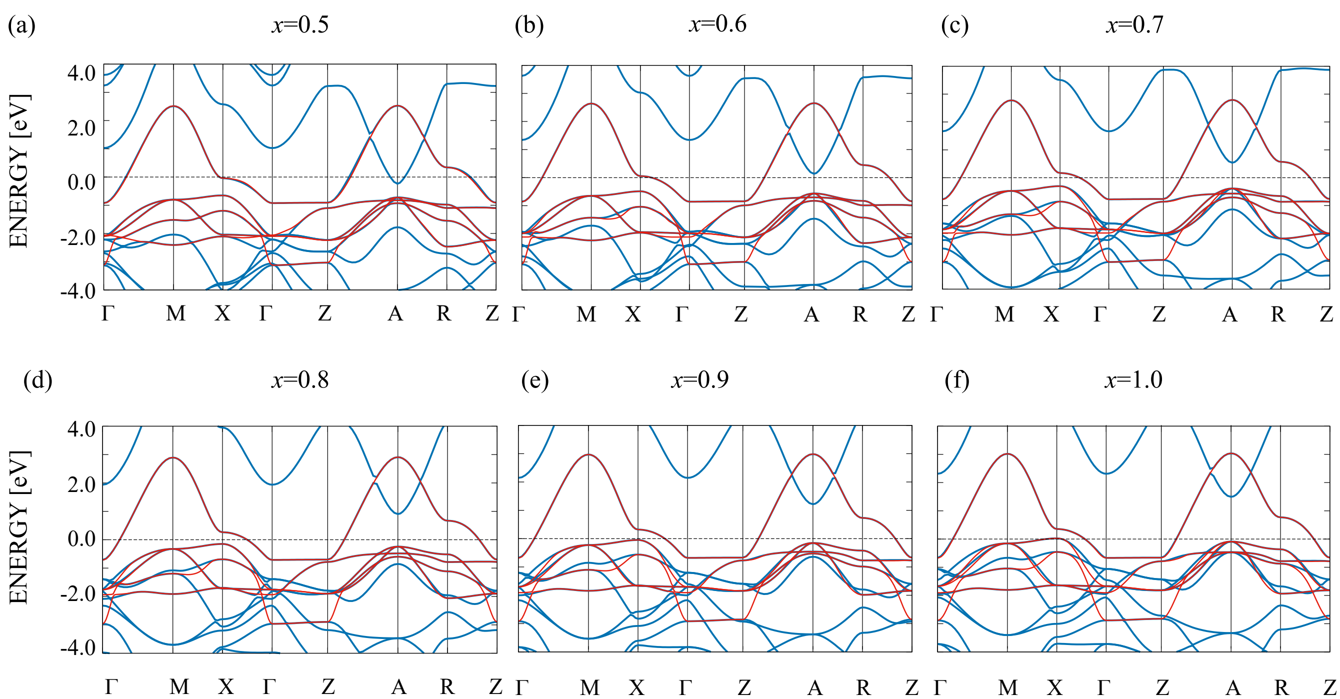

FIG. S4. The electronic band dispersion of $La_{1-x}Sr_xNiO_2$ obtained by GGA+U method with the in-plane lattice constant fixed to that of $SrTiO_3$. The substitution ratio x is written at the top of each panel. Here we have choosen the value of $U = 3.5$ eV and $J = 0.65$ eV, adopting the cRPA values. The blue lines indicate the first principles band dispersion, while the red lines are the band dispersion of the five-orbital model (Wannier interpolated).

region is advantageous for superconductivity for the GGA+U case.

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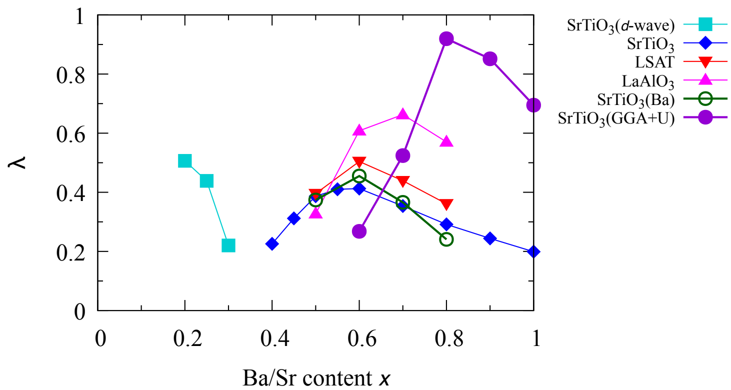

FIG. S5. The eigenvalue of the Eliashberg equation plotted against the Sr/Ba content x for the three substrates. The pairing symmetry having the largest λ is d-wave in the small x regime (calculated only for $SrTiO_3$ substrate), while it is $s\pm$-wave for $x > 0.3$. The purple filled circle indicate λ of the GGA+U case.