# 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 $\mathbf{LA_{1-x}SR_xNIO_2}$

In Fig. 1, 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.

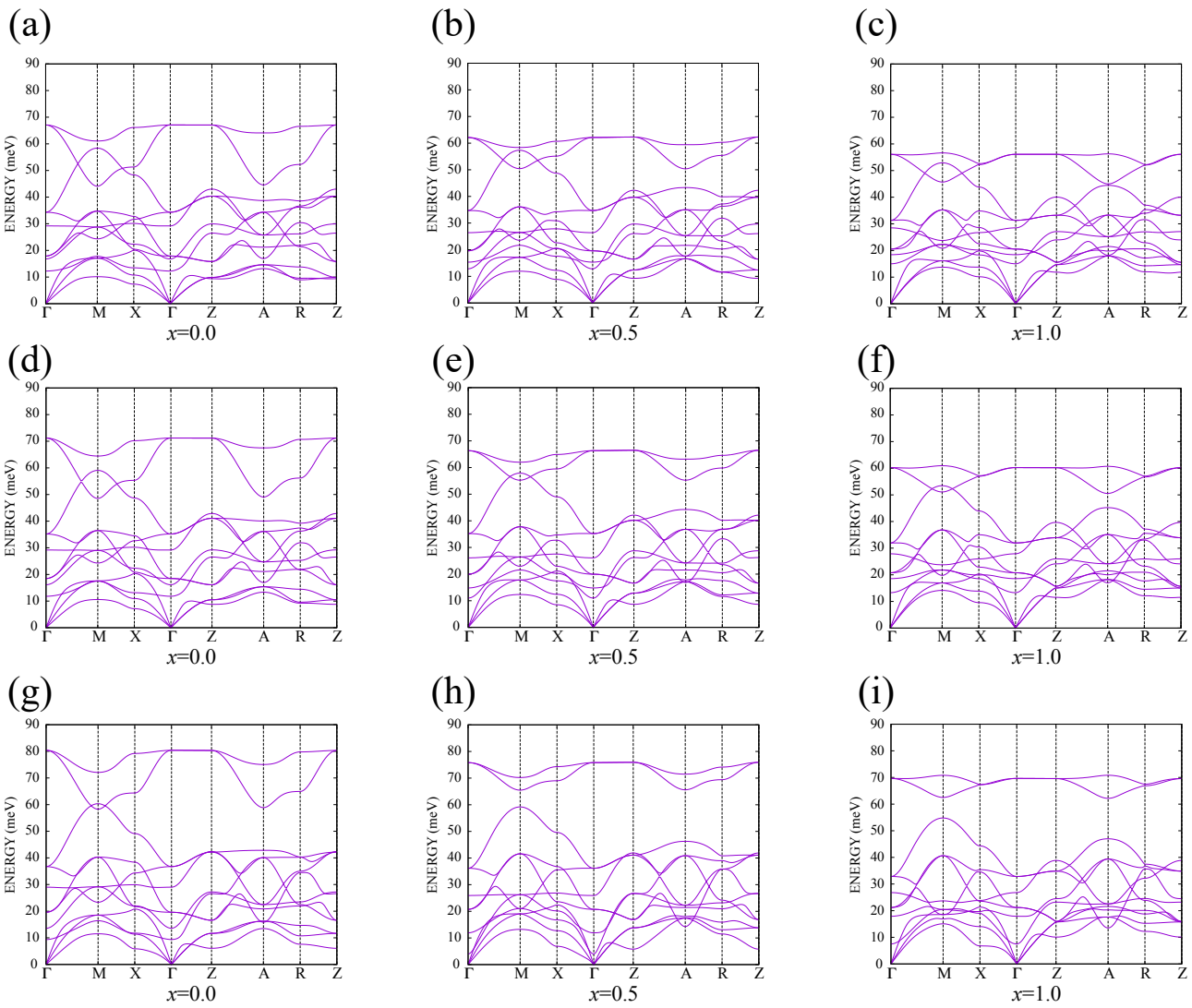


FIG. 1. The phonon dispersion of $La_{1-x}Sr_xNiO_2$ with the in-plane lattice constant fixed to that of $SrTiO_3$ ((a)-(c)), LSAT ((d)-(f)), or $LaAlO_3$ ((g)-(i)) substrates. The Sr content is $x = 0$ ((a),(d),(g)), $x = 0.5$ ((b),(e),(h)), or $x = 1$ ((c),(f),(i)).

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

In Fig. 2, 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 \sim$0.5–0.7 for $SrTiO_3$ and LSAT substrates and $x \sim$0.7 for $LaAlO_3$ substrate.

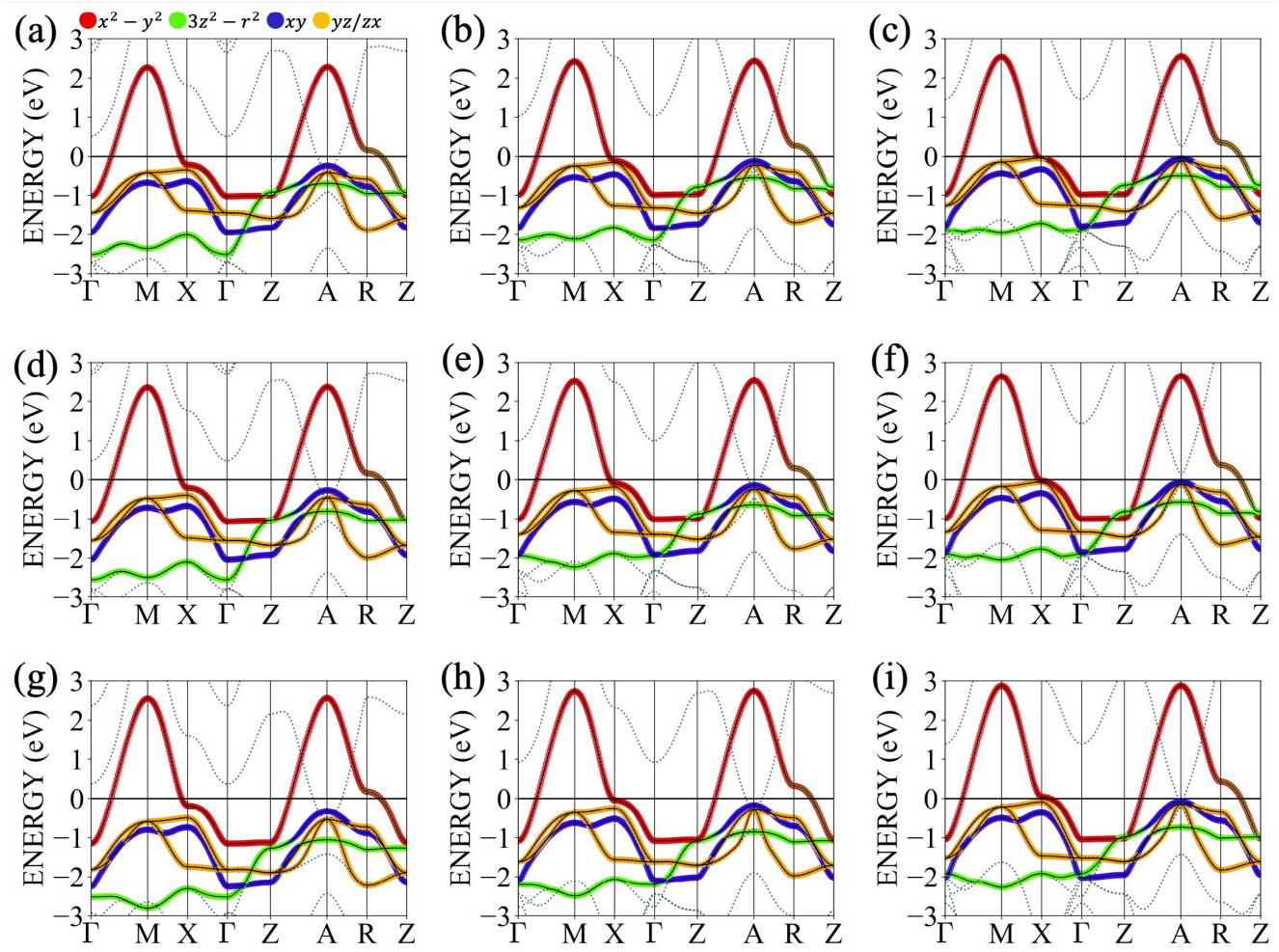


FIG. 2. The electronic band dispersion of $La_{1-x}Sr_xNiO_2$ with the in-plane lattice constant fixed to that of $SrTiO_3$ ((a)-(c)), LSAT ((d)-(f)), or $LaAlO_3$ ((g)-(i)) substrates. The Sr content is $x = 0.3$ ((a),(d),(g)), $x = 0.5$ ((b),(e),(h)), or $x = 0.7$ ((c),(f),(i)). The strength of the 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. 3(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. 3(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. 4, we show the band dispersion calculated by GGA+U method. Compared to Fig. 2, the band splittings between the $d_{x^2-y^2}$ orbital and the other orbitals are larger. In Fig. 5, we plot the eigenvalues $\lambda$ as a function of $x$ for comparison with GGA result. The change is probably caused by the change of the number of electrons. Namely, since the energy of the filled (not filled) orbitals is pushed up (down) from the Fermi level, the energy splitting between partially filled $d_{x^2-y^2}$ orbital and the nearly full-filled other orbitals is enlarged in GGA+U. This results in the increase in the number of electrons in the $d_{x^2-y^2}$ band, so that larger amount of holes are required to make the $d_{x^2-y^2}$ band

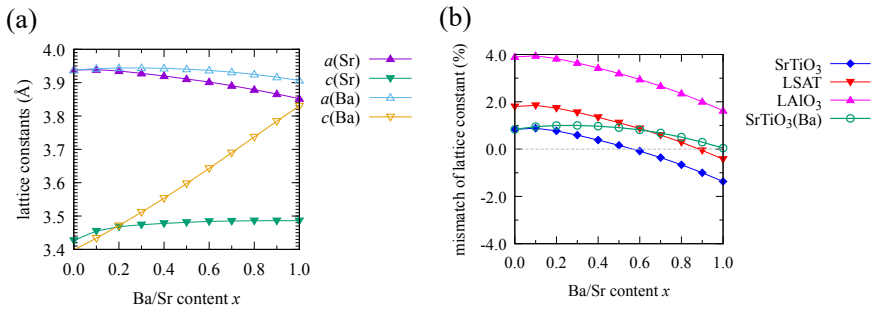


FIG. 3. (a) The lattice constants of $a$ and $c$ of $La_{1-x}AE_xNiO_2$($AE$ =Ba, Sr) against the ratio $x$ and (b) the mismatch of the lattice constants between the thin film and substrates. Here, the legends indicate the three substrates (with the lattice constants 3.905, 3.868, 3.790 Å for $SrTiO_3$, 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.

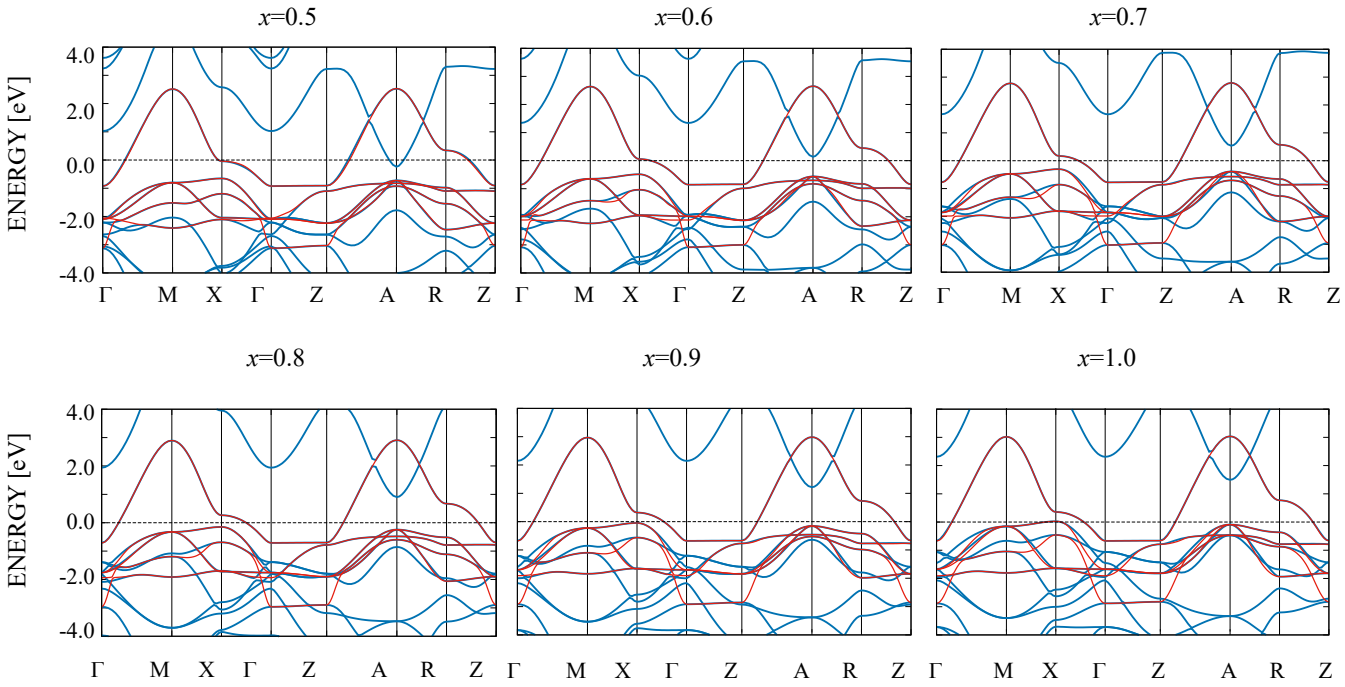


FIG. 4. The electronic band dispersion of $La_{1-x}Sr_xNiO_2$ obtained by GGA+U method with the in-plane lattice constant fixed to that of $SrTiO_3$. Here we have choosen the value of $U = 3.5$ eV and $J = 0.65$ eV, adopting the cRPA values. The blue lines indicate the first principles band dispersion, calculated in first-principles while the red lines are the band dispersion of the five-orbital model (Wannier interpolated).

incipient. This is the reason why higher doped region is advantageous for superconductivity for the GGA+U case.

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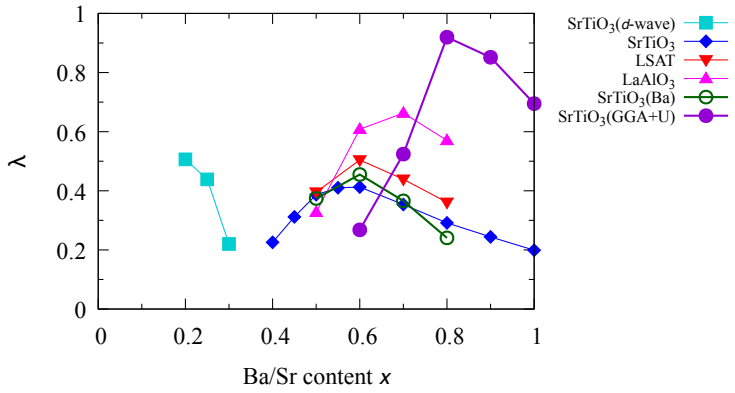


FIG. 5. The eigenvalue of the Eliashberg equation plotted against the Sr/Ba content $x$ for the three substrates. The pairing symmetry having the largest $\lambda$ is $d$-wave in the small $x$ regime (calculated only for $SrTiO_3$ substrate), while it is $s\pm$-wave for $x > 0.3$. The purple filled circle indicate $\lambda$ of the GGA+U case.