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.

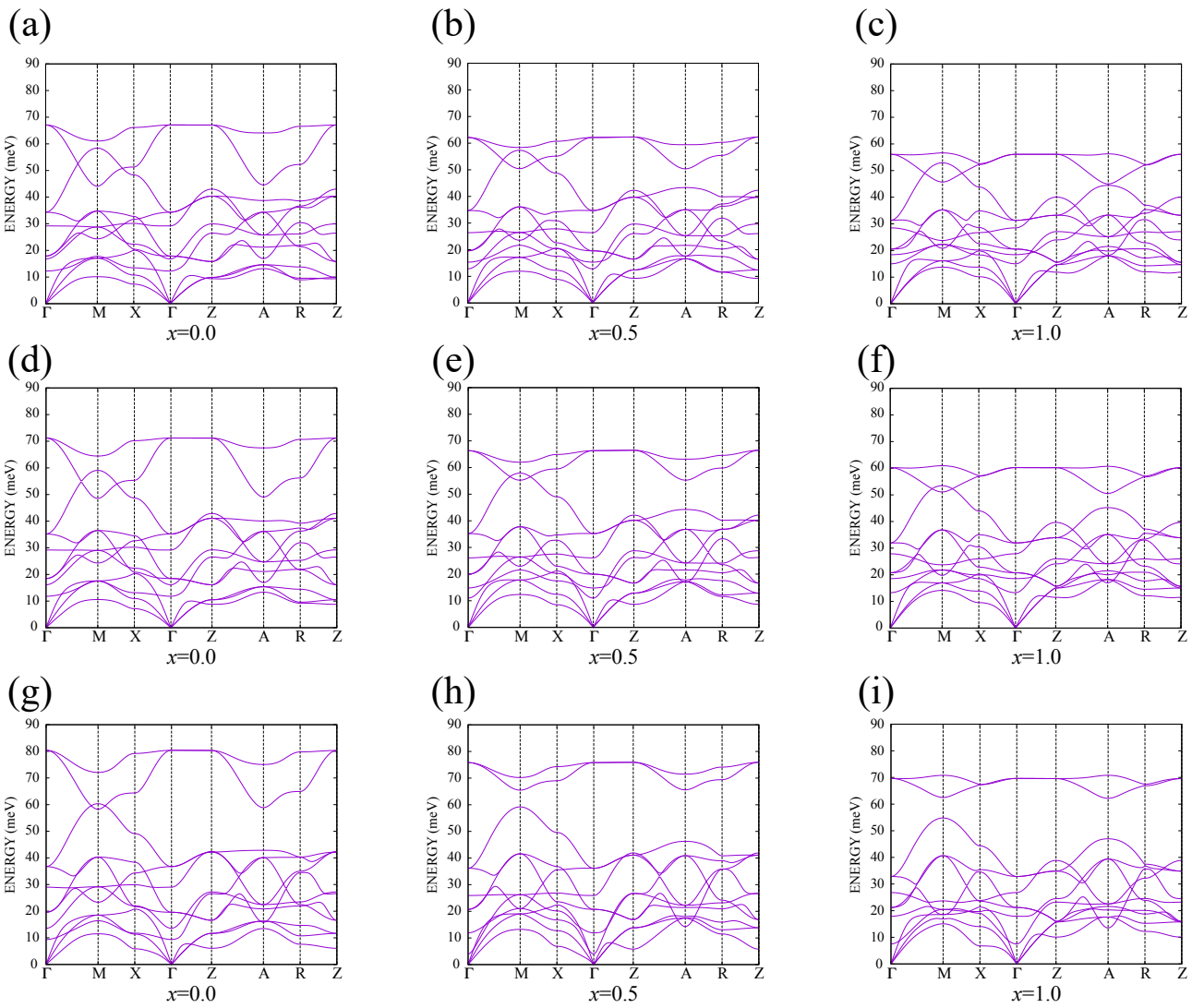

FIG. 1. The phonon dispersion of $La_{1-x}Sr_xNiO_2$ with the in-plane lattice constant fixed to that of $SrTiO_3$ ((a)-(c)), LSAT ((d)-(f)), or $LaAlO_3$ ((g)-(i)) substrates. The Sr content is $x = 0$ ((a),(d),(g)), $x = 0.5$ ((b),(e),(h)), or $x = 1$ ((c),(f),(i)).

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.

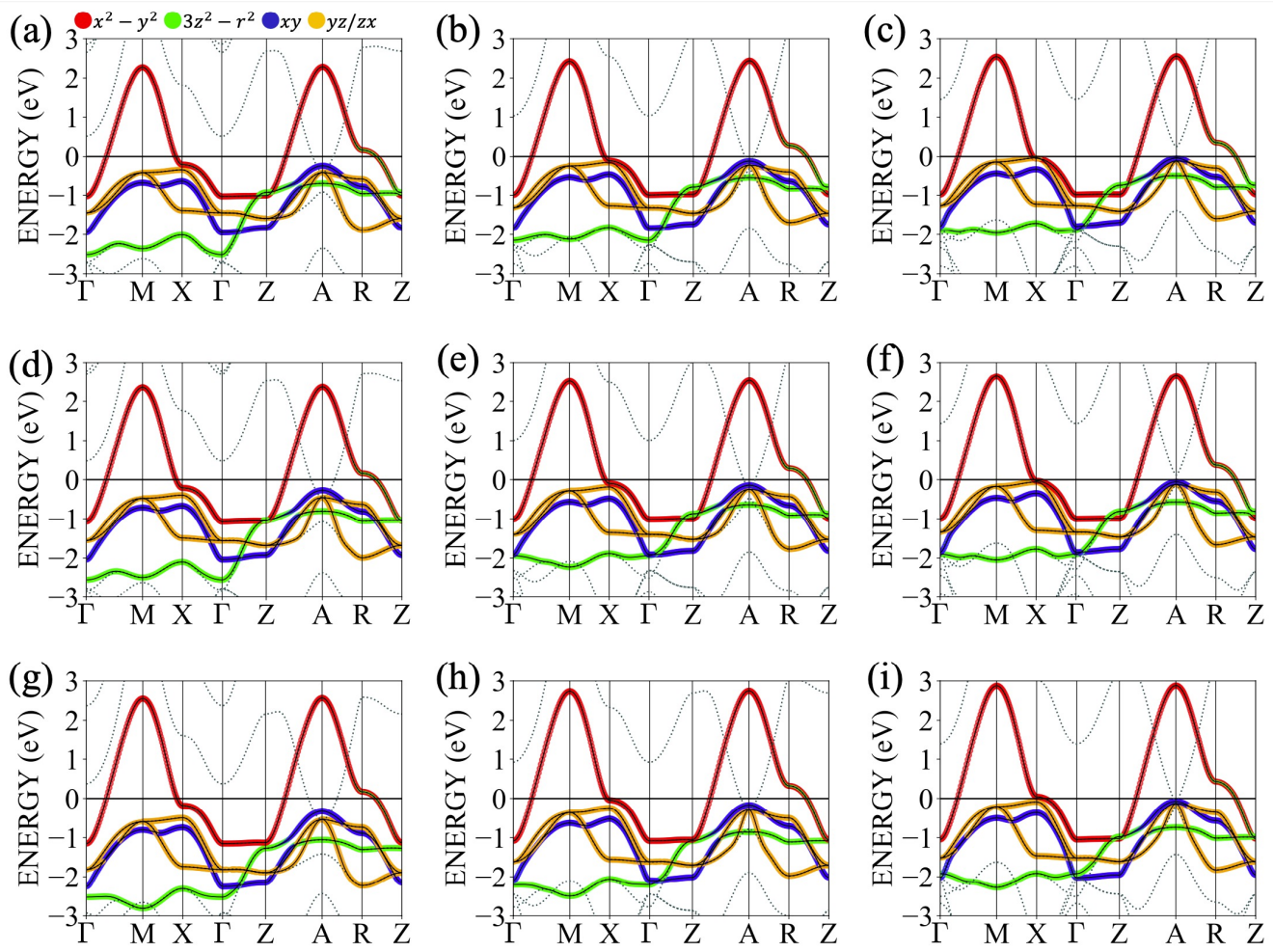

FIG. 2. The electronic band dispersion of $La_{1-x}Sr_xNiO_2$ with the in-plane lattice constant fixed to that of $SrTiO_3$ ((a)-(c)), LSAT ((d)-(f)), or $LaAlO_3$ ((g)-(i)) substrates. The Sr content is $x = 0.3$ ((a),(d),(g)), $x = 0.5$ ((b),(e),(h)), or $x = 0.7$ ((c),(f),(i)). The strength of the Wannier orbital characters are shown with the thickness of the color coded line.