Designing nickelate superconductors with $d^8$ configuration exploiting mixed-anion strategy

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Inspired by a recently proposed superconducting mechanism for a new cuprate superconductor Ba$_2$CuO$_2$δ, we theoretically design an unconventional nickelate superconductor with $d^8$ electron configuration. Our strategy is to enlarge the on-site energy difference between $3d_{xy}$ and $3d_{yz}$ orbitals by adopting halogens or hydrogen as out-of-plane anions, so that the $3d$ bands other than $d_{x^2-y^2}$ lie just below the Fermi level for the $d^8$ configuration, acting as incipient bands that enhance superconductivity. We also discuss a possible relevance of the present proposal to the recently discovered superconductor (Nd,Sr)NiO$_2$.

The two families of high-$T_c$ superconductors, cuprates and iron-based, are often contrasted as single-orbital vs. multiorbital systems. Namely, in the cuprates, only the $d_{x^2-y^2}$ orbital plays the main role while in the iron-based superconductors, $d_{xy}$, $d_{xz}$ and $d_{yz}$ orbitals largely contribute to the electronic structure around the Fermi level ($E_F$). Recently, however, there has occurred a possible paradigm shift to this picture, owing to some new experimental findings. One of such experiments is the discovery of high-$T_c$ superconductivity in Ba$_2$CuO$_2$δ, where the the apical oxygen height is so low that the energy levels of $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ can be reversed compared to conventional cuprates. Another example is a highly overdoped CuO$_2$ monolayer grown on Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, where $E_F$ is significantly lowered so that it reaches the $d_{3z^2-r^2}$ band $[5]$. For Ba$_2$CuO$_2$δ, various theoretical studies have been performed $[6,12]$, many of which treat multiorbital models. In Ref. $[12]$, two of the present authors have introduced a two-orbital model consisting of Wannier orbitals with $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ symmetries, where $s$-wave superconductivity with reversed gap sign between the two bands ($s^\pm$-wave pairing) is found to be strongly enhanced near half-filling when the energy level offset $\Delta E$ between $d_{3z^2-r^2}$ and $d_{x^2-y^2}$ orbitals is enlarged so that the bottom of the $d_{3z^2-r^2}$ band is positioned just above $E_F$. The strong enhancement of superconductivity was explained by transforming the two-orbital model to the bilayer Hubbard model, where the two orbitals of the former model correspond to the bonding and antibonding orbitals of the latter, and hence the orbital level offset $\Delta E$ in the former transforms to $2t_\perp$ in the latter with $t_\perp$ being the vertical hopping between the layers in the bilayer model. The bilayer Hubbard model has been intensively studied from the past $[13,29]$, and $s^\pm$-wave superconductivity is found to be strongly enhanced near half-filling when $t_\perp$ is several times larger than the in-plane hopping and $E_F$ lies in the vicinity of one of the bands $[13,18,22,28]$. Nowadays, a band sitting just below (or above) $E_F$ is often referred to as an incipient band, and has attracted interest in the study of iron-based superconductors $[34-37]$, bilayer and ladder-type lattices $[26,29,38,42]$, and flat band superconductivity $[42,46]$. The two-orbital to bilayer transformation is mathematically exact when there is no hybridization between the two orbitals and also $U = U' = J = J'$ is satisfied, where $U$, $U'$, $J$, and $J'$ are the intra-orbital repulsion, inter-orbital repulsion, Hund’s coupling, and the pair hopping interaction, respectively $[12,47]$. In reality, $U > U' > J$, $J'$ and the inter-orbital hybridization is present, but the analogy between the two models turns out to be approximately valid even in the realistic situation $[12]$. Actually, a situation where $E_F$ lies close to the $d_{3z^2-r^2}$ band edge is realized in a cuprate (La,Sr)$_2$CuO$_4$. One of the present authors and his colleagues have pointed out that the presence of the $d_{3z^2-r^2}$ band around $E_F$ is the origin of the suppression of $T_c$ of the $d$-wave superconductivity in this material $[45,51]$ due to the orbital component mixture around the antinodal regime. The difference between (La,Sr)$_2$CuO$_4$ and Ba$_2$CuO$_2$δ in Ref. $[12]$ is that in the former, the $e_g$ bands are close to $3/4$-filling on average (nearly two electrons in $d_{3z^2-r^2}$ and one electron in $d_{x^2-y^2}$), while the latter is closer to half-filling.

The above consideration brings us to an idea of realizing incipient-band-enhanced superconductivity in nickelates, where the $e_g$ bands become half-filled on average for the natural Ni$^{2+}$ valence, namely, the $d^8$ electron configuration. Actually, if all the bands other than $d_{x^2-y^2}$ sink below $E_F$ for the $d^8$ configuration, a pair of $d_{x^2-y^2}$ and any other $d$ orbital is half-filled (two electrons per two orbital on average), so if small amount of electrons are doped into such systems, we may expect enhanced $s^\pm$-wave superconductivity. To enlarge the energy level offset between $d_{3z^2-r^2}$ and $d_{3z^2-r^2}$ orbitals, we adopt a mixed-anion strategy $[52]$, namely, we chose halogens or hydrogens instead of oxygens as out-of-plane anions (which corresponds to enhancing $t_\perp$ in the bilayer system), for which we end up with the composition of $AE_2NiO_2X_2$ ($AE$=Ca,Sr, $X$=H, F, Cl, Br, I) $[53]$. We note that similar materials have been proposed in Ref. $[54]$ in the context of a recently discovered superconductor (Nd,Sr)NiO$_2$ $[55]$, but there, the aim was to...
construct ideal single band systems with $d^9$ electron configuration, where bands other than Ni $d_{x^2-y^2}$ do not intersect $E_F$ for the mother compound. In fact, here we later conversely discuss a possible relevance of the present $d^8$ proposal to the superconductivity of (Nd,Sr)NiO$_2$.

We consider $T$(K$_2$NiO$_4$) and $T'$ (Fig.1) structures as candidates for possible crystal structures. We also take La$_2$NiO$_4$ ($T$ structure) as a reference with $d^9$ configuration. We perform structural optimization adopting the PBE-GGA exchange-correlation functional and the projector augmented wave method. We use Vienna ab initio Simulation Package (VASP) and the Wien2k code. We adopt RKmax=7 for oxy-hydrides, and take 12 $k$ mesh and a plane-wave cutoff energy of 550 eV was used. After the structural optimization, we perform first-principles band-structure calculation using WIEN2k code. We adopt RKmax=7 (6 for oxy-hydrides), and take 12 $\times$ 12 $\times$ 12 $k$ mesh in the self-consistent-field calculations. From the calculated band structures, we extract the Wannier functions of five Ni 3d orbitals using the Wien2Wannier and Wannier90 codes. Throughout the study, the spin-orbit coupling is neglected.

In Fig.1(b), we plot the total energy difference between the two structures for all choices of $AE$ and $X$ elements. It is found that for $X=$Cl,Br and I, the $T$ structure has lower energy ($E_T - E_{T'} < 0$), while the difference between the two is small for $X=$H,F. In fact, phonon calculation of Ba$_{0.5}$La$_{0.5}$NiO$_2$F$_2$ in Ref. shows appearance of imaginary modes for the $T$ structure, but not for $T'$, which suggests stability of the latter. The optimized lattice constants presented in the supplemental material exhibit a trend where the in-plane lattice constant $a$ becomes larger as the ion radius of element $X$ or $AE$ is increased.

The first principles band structures obtained for the optimized lattice structures of La$_2$NiO$_4$ ($T$), Ca$_2$NiO$_2$Cl$_2$ ($T$), and Ca$_2$NiO$_2$H$_2$ ($T'$) are shown in Fig.2. The energy dispersion of the five orbital model is superposed to the first principles bands for each material. The band structures of materials with other elements are presented in the supplemental material. It can be noticed that in the mixed-anion materials, the $d_{x^2-y^2}$ band totally sinks below $E_F$ despite the $d^9$ electron configuration with the $d_{x^2-y^2}$ band partially filled, in sharp contrast to the case of La$_2$NiO$_4$. The entire $d_{xy}$ band also lies below $E_F$, while the top of $d_{xz/yz}$ bands intersects $E_F$.

In Fig.2, we plot the on-site energy ($\Delta E$) of the $d$ orbitals with respect to that of $d_{x^2-y^2}$ in the five orbital model. Let us focus on the crystal structure having the lower total energy (denoted by the solid symbols). $|\Delta E|$ tends to be larger (i.e., the energy level is lowered since $\Delta E < 0$) as the ion radius of $X$ is reduced within $X=$ Cl, Br and I. This is due to the smaller in-plane lattice constant (shorter Ni-O distance), which pushes up the $d_{x^2-y^2}$ energy level. For the $T'$ structure, the on-site energy of the $d_{3z^2-r^2}$ orbital is strongly reduced due to the absence of the apical anions, but the $t_{2g}$ orbitals are pushed up compared to those in the $T$ structure. If we compare $AE=$Ca and Sr, $|\Delta E|$ of the $t_{2g}$ orbitals are reduced in the former compared to the latter, while that of $d_{x^2-y^2}$ is less affected. This is because the lattice constants $a$ and $c$ are shorter for $AE=$Ca than for Sr.

We now analyze superconductivity based on the obtained five-orbital models. We assume on-site intra- and inter-orbital interactions, $U$, $U'$, $J$, and $J'$, and the many-body study of this model is performed within the fluctuation exchange approximation (FLEX). We mainly adopt $U = 4$eV, $J = J' = U/8$, $U' = U - 2J$, but also discuss the interaction dependence in the supplemental material. A relatively large $U$ is taken in accord with a study for LaNiO$_2$. We obtain the renormalized Green’s function by solving the Dyson’s equation in a self-consistent calculation. The obtained Green’s function and the pairing interaction mediated mainly by spin-fluctuations are plugged into the linearized Eliashberg equation. Since the eigenvalue of the equation reaches unity at $T_c$, here we adopt $\lambda$, obtained at a fixed temperature of $T = 0.01$eV, to measure how close the system is to superconductivity. The eigenfunction of the Eliashberg equation will be called the gap function. In the FLEX calculation, $16 \times 16 \times 4$ ($k_x, k_y, k_z$) mesh and 2048 Matsubara frequencies were taken.
consisting only of $d_{x^2-y^2}$, indicating the important role played by the incipient $d_{x^2-y^2}$ bands. On the other hand, adding $d_{xy}$ and/or $d_{3z^2-r^2}$ orbitals to the $d_{x^2-y^2} + d_{x^2+y^2}$ model does not strongly affect $\lambda$. Our interpretation is that the interaction between $d_{xy}$ (or $d_{3z^2-r^2}$) and $d_{x^2-y^2}$ orbitals enhances superconductivity because the signs of the gap are opposite, but the interaction between $d_{xy}$ (or $d_{3z^2-r^2}$) and $d_{x^2+y^2}$ gives negative contribution to superconductivity because of the same sign of the gap. Since $\lambda$ is dominated by the position of the $d_{xz}/y^2$ bands, the materials having larger energy difference between $d_{x^2-y^2}$ and $d_{xz}/y^2$ orbitals, corresponding to larger $t_\perp$ in the bilayer Hubbard model [12], tend to exhibit larger $\lambda$. On the other hand, it should be stressed that the strong reduction of $\lambda$ for La$_2$NiO$_4$ compared to mixed-anion materials mainly comes from the the small $|\Delta E|$ for the $d_{xz}/y^2$ orbital; the $d_{x^2-y^2}$ band intersecting $E_F$ gives rise to strong development of low energy spin fluctuations, which works destructively against superconductivity, as in the case of the bilayer Hubbard model with small $t_\perp$ [24, 25, 27, 28]. Further analysis on the role played by each orbital is given in the supplemental material [68].

We note that all of our calculations assume low-spin state, while nickelates with $d^8$ configuration can take high-spin states when the $d$-level splittings are small. In fact, the reference system in our study La$_2$NiO$_4$ is actually well known to be in the high-spin state, and also

In Fig. 3(a)(b), we plot the eigenvalue of the Eliashberg equation against the band filling, varied assuming rigid band, for various materials with the crystal structure ($T$ or $T'$) having lower total energy. In all mixed-anion compounds, $\lambda$ is peaked at around $n = 4.1$ to 4.2, which corresponds to 10 to 20% electron doping starting from the stoichiometric band filling of $n = 4$. The compounds having the largest maximum $\lambda$ are Ca$_2$NiO$_2$Cl$_2$ and Ca$_2$NiO$_2$H$_2$. These maximum values of $\lambda$ are much larger compared to that of La$_2$NiO$_4$ [73], and they are in fact even larger than that of HgBa$_2$CuO$_4$, a $T_c = 100K$ superconductor, obtained in the same manner [73]. It is also worth mentioning that the Stoner factor for magnetic ordering remains far from unity for the situation when $\lambda$ of superconductivity is optimized, which is typical for the incipient-band enhanced superconductivity (see supplemental material [68]).

The gap function presented in Fig. 3(c) for the case of Ca$_2$NiO$_2$Cl$_2$ with $n = 4.125$ shows that the four bands other than $d_{x^2-y^2}$ have the same sign of the gap, opposite to that of the $d_{x^2-y^2}$ band (see the supplemental material for the contour plot of the gap [68]). In this sense, this is $s\pm$-wave pairing with the four bands other than $d_{x^2-y^2}$ being incipient, namely, located below $E_F$, with the $d_{xz}/y^2$ band top being the closest to $E_F$. In order to see the role played by each orbital in more detail, we extract one, two, three, or four orbitals from the five orbital model, and apply FLEX to those multiorbital models to obtain $\lambda$ in a similar manner. From Fig. 3(d), it can be seen that $\lambda$ in the $d_{x^2-y^2} + d_{x^2+y^2}$ model is strongly enhanced compared to the single orbital model.
Sr$_2$NiO$_2$Cl$_2$, synthesized in Ref.[71], was found to be in a high-spin state. On the other hand, a hypothetical infinite layer nickelate SrNiO$_2$, without apical anions, was theoretically shown to have a low-spin ground state [72]. Hence, large $|\Delta E|$ is not only preferable for enhancing $T_c$, but it is also favorable from the viewpoint of realizing a low-spin ground state. In this sense, $AE$=Ca rather than Sr and also $X$=Cl rather than Br or I (T structure), is likely to be the best choice from the viewpoint of both realizing a low-spin state and enhancing $T_c$ because of the smaller in-plane lattice constant and hence larger $|\Delta E|$. Our result indicates that superconductivity in $AE_2NiO_2X_2$ is optimized by electron doping, which may be realized in actual materials by, e.g., partially substituting Ca$^{2+}$ (or Sr$^{2+}$) with La$^{3+}$. In fact, a pure $d^9$ configuration (band filling of $n=4$) may result in an insulating state not predicted within the present calculation. Electron doping should prevent the material from being an insulator, and hence may also stabilize the preferred low-spin state in actual materials. In total, the materials we propose here as candidates for new unconventional superconductors have the composition form Ca$_{2-x}$La$_x$NiO$_2$Cl$_2$ and Ca$_{2-x}$La$_x$NiO$_2$H$_2$.

Now, if we increase the amount of electron doping in the present materials, they approach the materials with $d^9$ electron configuration studied in Refs.[74, 77] in the context of a recently discovered superconductor (Nd,Sr)NiO$_2$ [75]. Then, conversely, it is interesting to see how the $d^9$ and $d^{8}$ states are connected in (Nd,Sr)NiO$_2$ by hypothetically removing the electrons. Here we consider LaNiO$_2$ adopting the experimentally determined lattice parameters of NdNiO$_2$ to avoid the ambiguity regarding the treatment of the $f$ electrons in Nd [76]. Since a previous study has shown that the La 5$d$ orbitals have small effect on spin-fluctuation-mediated superconductivity [74], we construct a five Ni-3$d$-orbital model similar to those for $AE_2NiO_2X_2$, as shown in Fig. 5(a). The band structure somewhat resembles that of $AE_2NiO_2Cl_2$ in that the position of the $d_{3z^2-r^2}$ band is lowered, which is because the apical anions are absent in this infinite layer material, but the difference lies in that the $d_{3z^2-r^2}$ band exhibits strong three dimensionality. We perform similar FLEX analysis of superconductivity for this model by hypothetically varying the band filling assuming a rigid band. As expected from our results on $AE_2NiO_2X_2$, there appears a peak in $\lambda$ close to $n=4$, i.e., the $d^8$ configuration, in addition to the already known $d$-wave superconductivity around $n=4.5$, the $d^9$ configuration.

Although we believe that the mechanism similar to the cuprates, where only the $d_{x^2-y^2}$ band plays an important role, is a strong candidate for the superconducting mechanism of (Nd,Sr)NiO$_2$, the present analysis suggests that their might be an alternative scenario where Ni 3$d$ orbitals other than $d_{x^2-y^2}$ play the role of incipient bands. In fact, as studied in Ref.[78], (Nd,Sr)NiO$_2$H may form during the reduction process by CaH$_2$, which would reduce the number of $d$ electrons [80]. Another theoretical study shows that similar situation can occur also at the SrTiO$_3$ substrate interface [81]. It will then be an interesting future problem to carefully examine the Ni valence in (Nd,Sr)NiO$_2$. Also, the gap function would be of interest since $d$-wave should be realized for the $d^9$ pairing mechanism, whereas $s$-wave is expected for the $d^8$ scenario. In fact, while finalizing the present paper, a tunneling spectroscopy experiment has been reported [82], where $s$-wave and $d$-wave-like gaps have been observed, depending on the position on the sample. The experiment has been interpreted in terms of the gap with different symmetry opening on different Fermi surfaces, which was suggested theoretically [83].

From our viewpoint, the position dependence of the pairing symmetry might originate from the inhomogeneity of the residual hydrogen remained during the reduction process [84].

To conclude, we have designed unconventional nickelate superconductors with nearly $d^9$ electron configuration, where superconductivity is enhanced by the bands other than $d_{x^2-y^2}$ playing a role of the incipient bands. The key idea is to exploit the mixed-anion strategy to enlarge the on-site energy difference between $d_{x^2-y^2}$ and other $d$ orbitals. This corresponds to increasing the interlayer hopping $t_{\perp}$ of the bilayer Hubbard model, which is known to exhibit $s \pm$-wave superconductivity strongly enhanced by the incipient-band effect for large $t_{\perp}$. Possible relevance of the present proposal to the observation of superconductivity in (Nd,Sr)NiO$_2$ is an interesting future problem, where a non-rigid-band variation of the incipient-band dispersion due to residual hydrogen should be taken into account.

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Supplemental material: Designing nickelate superconductors with $d^8$ configuration exploiting mixed-anion strategy

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LATTICE CONSTANTS AND BAND STRUCTURES

In Fig S1 and Figs S2-S5 we plot the lattice constants obtained by structural optimization and the corresponding band structures, respectively, for all the materials considered in the present study. The lattice constants are larger for $AE$ and/or $X$ with larger ionic radius, except for the case of H in the $T$ structure. As for the band structures, the relative position between the bands reflects the tendency seen in the on-site energy of each orbital (Fig.3 of the main text).

DEPENDENCE ON THE INTERACTIONS

Here, we vary the interaction values in the five orbital model of Ca$_2$NiO$_2$Cl$_2$ in various manners and see how the eigenvalue of the Eliashberg equation is affected. In Fig S6(a), the interactions are varied maintaining $U’ = U - 2J$ so as to satisfy orbital-rotation symmetry. Within the varied parameter range, larger $U$ results in a suppression (slight enhancement) of superconductivity for $n < 4.2$ ($n > 4.2$). From Fig S6 (b) to (d), one of $U$, $U’$, $J$, $J’$ is varied, while others are fixed. The overall tendency is that increasing $U’$ and $J’$ enhances superconductivity, while increasing $U$ and $J$ degrades it.
FIG. S4. Similar figure as in Fig. S2 with $AE=$Sr and the $T$ structure.

FIG. S5. Similar figure as in Fig. S2 with $AE=$Sr and the $T'$ structure.

**STONER FACTOR FOR MAGNETIC ORDERING**

The tendency toward magnetic ordering can be measured by calculating the Stoner factor within FLEX. In the spin-fluctuation mediated superconductivity, the Stoner factor typically becomes very close to unity (larger than 0.95, where the Stoner factor = 1 signals magnetic ordering) as the eigenvalue of the Eliashberg equation increases, which indicates that superconductivity and antiferromagnetism closely compete with each other [S1]. It is known that this is not the case for the $s\pm$-wave superconductivity enhanced by the incipient band [S2] because the incipient-band mechanism exploits finite energy spin fluctuations. In fact, for the five orbital model of the proposed materials, the Stoner factor remains away from unity in the parameter regime where superconductivity is optimized. As a typical example, in Fig. S7 we plot the Stoner factor calculated for the five orbital model of Ca$_2$NiO$_2$Cl$_2$ with $U = 4$eV, $J = J' = U/8$, $U' = U - 2J$, and $T = 0.01$eV.

**GAP FUNCTION**

In Fig. S8 we show the contour plot of the gap function for the five orbital model of Ca$_2$NiO$_2$Cl$_2$. As already seen in Fig. 4(c) of the main text, this is an $s\pm$-wave pairing with small $k$ dependence of the gap, where the gap changes sign between the $d_{x^2-y^2}$ and incipient $d$ orbitals. For La$_2$NiO$_4$, there is no chance for superconductivity since $\lambda$ is small, and, in the first place, we assume an unrealistic low-spin state. Nonetheless, we plot the inter-
FIG. S8. Contour plot of the gap function of the five orbital model of Ca$_2$NiO$_2$Cl$_2$ for $n = 4.125$. Only the orbital-diagonal components are shown.

FIG. S9. Contour plot of the gap function of the five orbital model of La$_2$NiO$_4$ for $n = 4.125$. Here, we plot the off-diagonal component since it has appreciable amplitude.

ORBITAL DECOMPOSITION

In Fig.4(d) of the main text, we have only considered models that contain the $d_{xz/yz}$ orbitals (except for the single orbital model). The reason for this is as follows. Since the top of the $d_{xz/yz}$ bands has the highest energy among the bands other than $d_{x^2-y^2}$ and the Fermi level for the stoichiometric band filling of $n = 4$ intersects only the $d_{x^2-y^2}$ and $d_{xz/yz}$ bands, the Fermi level of the full five orbital model with the band filling of $n \geq 4$ is the same as that of an $n_{orb}$ orbital model with the band filling of $n - (5 - n_{orb})$, as far as the models that contain the $d_{xz/yz}$ orbitals are concerned. Conversely, the Fermi level of, say, a two-orbital $d_{x^2-y^2} + d_{xy}$ model with the band filling of $n - 3$ is not the same as that of the full five orbital model with the band filling of $n$. Hence, such models were not considered in the main text. Nonetheless, it is interesting to study how each band would affect superconductivity if other bands were absent. In Fig. S10, we plot the eigenvalue of the Eliashberg equation against the band filling for two-orbital $d_{x^2-y^2} + d_{xy}$ and $d_{x^2-y^2} + d_{3z^2-r^2}$ models, in addition to the $d_{x^2-y^2} + d_{xz/yz}$ model, the single orbital $d_{x^2-y^2}$ model, and the full five orbital model. It can be seen that all of the bands can act as an incipient band that enhances $s\pm$ superconductivity compared to the single orbital case. A tendency here is that the orbitals having larger $|\Delta E|$ (level offset with respect to the $d_{x^2-y^2}$ orbital, corresponding to $2t_\perp$ in the bilayer Hubbard model) give stronger enhancement of superconductivity, and superconductivity is optimized at lower band fillings. This tendency is indeed the same as that seen in the bilayer Hubbard model[S4, S5].

[S1] See, e.g., R. Arita, K. Kuroki, and H. Aoki, J. Phys. Soc. Jpn. 69, 1181 (2000). Here $1/\chi$ is plotted against the temperature, where $\chi$ is the FLEX spin susceptibility. Stoner factor is given by $1 - 1/\chi$. Note that the Stoner factor exhibits a much weaker temperature dependence compared to the eigenvalue of the Eliashberg equation $\lambda$. This is also the case for systems with incipient bands.

[S2] D. Ogura, Springer Theses, "Theoretical Study of Electron Correlation Driven Superconductivity in Systems with Coexisting Wide and Narrow Bands", Springer (2019).

[S3] K. Yamazaki, M. Ochi, D. Ogura, K. Kuroki, H. Eisaki, S. Uchida, and H. Aoki, arXiv:2003.04015

FIG. S10. $\lambda$ against the band filling for various models of Ca$_2$NiO$_2$Cl$_2$. 

[S4] D. Ogura, Springer Theses, "Theoretical Study of Electron Correlation Driven Superconductivity in Systems with Coexisting Wide and Narrow Bands", Springer (2019).
[S4] T. Maier and D.J. Scalapino, Phys. Rev. B 84, 180513(R) (2011).
[S5] K. Matsumoto, D. Ogura and K. Kuroki, J. Phys. Soc. Jpn. 89, 044709 (2020).
[S6] D. Kato and K. Kuroki, Phys. Rev. Research. 2, 023156 (2020).