Supplementary Information for "Origin of the Diagonal Double-Stripe Spin-Density-Wave and Potential Superconductivity in $La_3Ni_2O_7$ at Ambient Pressure"

Yu-Bo Liu,[1,*] Hongyi Sun,[2,3,*] Ming Zhang,[4,*] Qihang Liu,[5,6] Wei-Qiang Chen,[5,6,†] and Fan Yang[1,‡]

[1] *School of Physics, Beijing Institute of Technology, Beijing 100081, China*
[2] *Shenzhen Institute for Quantum Science and Engineering, Southern University of Science and Technology, Shenzhen 518055, China*
[3] *International Quantum Academy, Shenzhen 518048, China*
[4] *Zhejiang Key Laboratory of Quantum State Control and Optical Field Manipulation, Department of Physics, Zhejiang Sci-Tech University, 310018 Hangzhou, China*
[5] *Department of Physics, Southern University of Science and Technology, Shenzhen 518055, China*
[6] *Shenzhen Key Laboratory of Advanced Quantum Functional Materials and Devices, Southern University of Science and Technology, Shenzhen 518055, China*

I. THE DFT BAND AND THE TIGHT-BINDING MODEL FOR $LA_3NI_2O_7$ UNDER HIGH PRESSURE

This section presents the results of the density-functional-theory (DFT) and tight-binding (TB) models for $La_3Ni_2O_7$ under high pressure (HP). The DFT calculations for the HP phase are similar to those for the ambient pressure (AP) phase as described in the main text, except that we start from the high pressured (29.5 Gpa) crystal structure with the measured lattice constants [1] and set the Kmesh to be $13 \times 13 \times 12$ to sample the Brillouin zone of the primitive unit cell. The obtained DFT band structure is shown in Fig. S1(a).

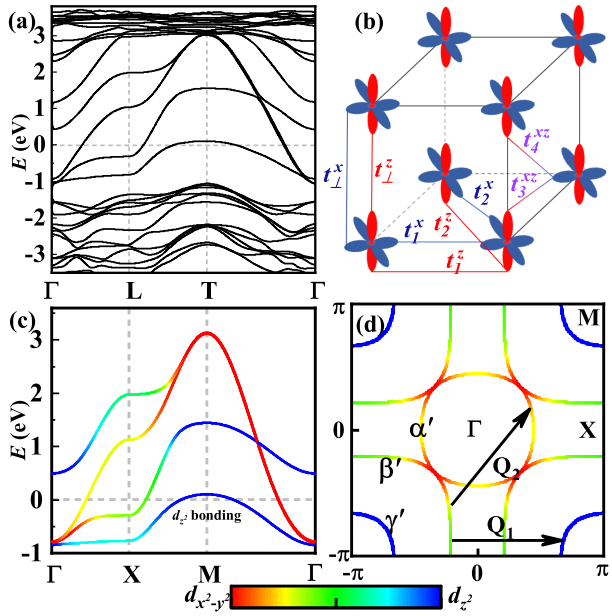

FIG. S1. (color online) The DFT band structure and four-band TB model for $La_3Ni_2O_7$ under HP. (a) The DFT band structure, with experimental refined lattice constants adopted. (b) Schematic of the hopping integrals for the bilayer four-band TB model. The red(bule) orbitals represent Ni-d_{z^2}(-$d_{x^2-y^2}$) orbitals. (c) The TB band structure along the high symmetry lines. (d) the FS in the BZ, marked by α', β' and γ'. The color in (c-d) indicates the orbital weight of d_{z^2} and $d_{x^2-y^2}$.

* These three authors contributed equally to this work.
† chenwq@sustech.edu.cn
‡ yangfan_blg@bit.edu.cn

TABLE S1. The value of four-band TB hopping parameters for $La_3Ni_2O_7$ under HP. In the superscript and subscript, $x(z)$ represents the $d_{x^2-y^2}(d_{z^2})$ orbit, $\perp$ represents interlayer hopping, and $1, 2$ represents the NN and NNN hopping, respectively. ϵ is on-site energy. The unit of all parameters is eV.

t_1^x	t_2^x	$t_\perp^x$	t_3^{xz}	ϵ_x
-0.490	0.073	0.008	0.244	0.512
t_1^z	t_2^z	$t_\perp^z$	t_4^{xz}	ϵ_z
-0.119	-0.017	-0.670	-0.031	0

Focusing on the $3d$-E_g orbitals of Ni atoms, similarly to the case of AP, we construct a bilayer two-orbital TB model. The TB Hamiltonian can also be expressed as Eq. (1) in the main text, with the hopping integrals $t_{ij,\mu\nu}$ are provided in Tab. S1 and Fig. S1(b). For $La_3Ni_2O_7$ under HP, since the apical Ni-O-Ni bond approaches 180°, each Ni atom within the layer is in an identical environment. The unit cell contains one Ni atom per layer, ultimately resulting in a four-band TB model.

In Fig. S1(b), all the hopping integrals $t_{ij,\mu\nu}$ are illustrated. Here, the red, blue, and purple lines represent the hopping on the d_{z^2} orbital, the $d_{x^2-y^2}$ orbital, and between two orbitals, respectively. The corner mark x/z indicates $d_{x^2-y^2}/d_{z^2}$- orbitals, $1/2$ indicates nearest-neighbor (NN) /next-nearest-neighbor (NNN) intralayer hopping, and $\perp$ means interlayer hopping. The values of all the hopping integrals are listed in Tab. S1.

Fig. S1(c) shows the bands obtained from the TB model, which successfully capture the essential characteristics of the DFT bands. We notice that the d_{z^2}-orbital bonding band crosses the Fermi energy. The corresponding Fermi surfaces (FSs) are shown in Fig. S1(d). There are three pockets, including an electron pocket α', an hole pocket β', and a hole pocket γ', in which the pocket γ' is almost entirely contributed by the d_{z^2}-orbital. Interestingly, there are several FS-nestings. The FS-nesting between α' and β' pockets is marked as $\boldsymbol{Q}_2$, which qualitatively corresponds to the nesting vector $\boldsymbol{Q}$ for AP as shown in Fig. 3(b) in the main text. The FS-nesting between α' and γ' pockets, marked as $\boldsymbol{Q}_1$, is considered to contribute significantly to SC[2, 3].

II. THE TB HOPPING INTEGRALS FOR $LA_3NI_2O_7$ AT AMBIENT PRESSURE

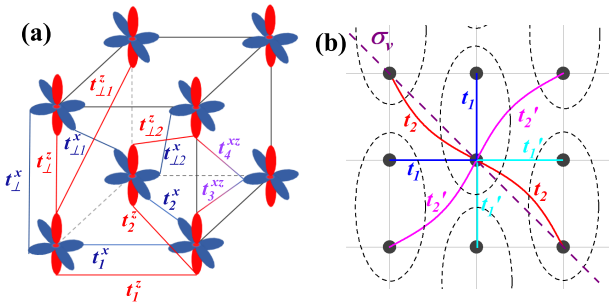

FIG. S2. (color online) Schematic of the hopping integrals for $La_3Ni_2O_7$ at AP. (a) Schematic of the main hopping integrals for the eight-band TB model, in which the third-nearest-neighbor hopping integrals ($t_3^{x/z}$ in Tab. S2) are not shown. For $La_3Ni_2O_7$ at AP, the hoping integrals along different directions may be different, but for brevity, they are represented by the same symbol in (a). (b) All the NN and NNN hoping integrals in (a) along different directions. Based on the lattice symmetry, the NN hopping integrals t_1(or NNN hopping integrals t_2) can be divided into two sets, labeled as t_1 and t_1' (or t_2 and t_2'). The gray dots and dashed ovals represent Ni atoms and the unit cell in the a-b plane, respectively. σ_v represents the mirror inversion symmetry of the lattice.

This scetion provides the TB hopping parameters for $La_3Ni_2O_7$ at AP. The hopping integrals $t_{ij,\mu\nu}$ up to NNN are illustrated in Fig. S2(a), with the corner marks having the same meaning as in Tab. S1. For $La_3Ni_2O_7$ at AP, the planform of lattice is shown in Fig. S2(b), the lattice lacks D_4 point group symmetry but has the mirror inversion symmetry σ_v. Based on the lattice symmetry, the four NN hopping integrals t_1(or NNN hopping integrals t_2) can be divided into two sets, labeled as t and t', as shown in Fig. S2(b). The dashed ovals represent a unit cell. The values of all the hopping integrals are listed in Tab. S2.

TABLE S2. The value of eight-band TB hopping parameters for $La_3Ni_2O_7$ at AP. The meaning of each superscript and subscript is the same as Tab. S1. The unit of all parameters is eV.

	t_1^x	t_2^x	t_3^x	$t_\perp^x$	$t_\perp^{x1}$	$t_\perp^{x2}$
t	-0.403	0.045	-0.060	0.018	-0.010	0.011
t'	-0.398	0.058			-0.010	0.011
	t_1^z	t_2^z	t_3^z	$t_\perp^z$	$t_\perp^{z1}$	$t_\perp^{z2}$
t	-0.076	-0.013	-0.012	-0.597	0.013	0.009
t'	-0.104	-0.016			0.012	0.008
	t_3^{xz}	t_4^{xz}	ϵ_x	ϵ_z		
t	0.211	-0.022	0.558	0		
t'	0.190	-0.025				

[1] H. Sun, M. Huo, X. Hu, J. Li, Z. Liu, Y. Han, L. Tang, Z. Mao, P. Yang, B. Wang, J. Cheng, D.-X. Yao, G.-M. Zhang, and M. Wang, Signatures of superconductivity near 80 K in a nickelate under high pressure, Nature **621**, 493 (2023).

[2] Q.-G. Yang, D. Wang, and Q.-H. Wang, Possible $s_\pm$-wave superconductivity in $La_3Ni_2O_7$, Phys. Rev. B **108**, L140505 (2023).

[3] Y.-B. Liu, J.-W. Mei, F. Ye, W.-Q. Chen, and F. Yang, $s^\pm$-wave pairing and the destructive role of apical-oxygen deficiencies in $La_3Ni_2O_7$ under pressure, Phys. Rev. Lett. **131**, 236002 (2023).