

ADDENDUM

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# Addendum: Fermiology and electron dynamics of trilayer nickelate $\text{La}_4\text{Ni}_3\text{O}_{10}$

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## Supplementary Note 4 | Structural information of the DFT calculation

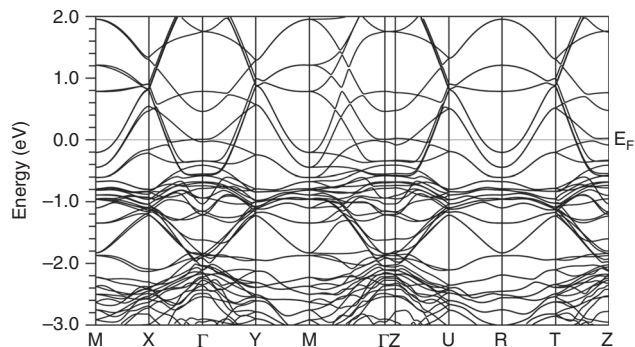
The DFT calculations in the main text use crystal structure information determined by x-ray diffraction (XRD) measurements of  $\text{La}_4\text{Ni}_3\text{O}_{10}$ . The room temperature XRD measurements on all samples were consistent with mixed phases of orthorhombic and monoclinic symmetry. However, the in-plane lattice constants of these two phases differ by <1%, leading to minimal influence on band structure calculations. Furthermore, any impact on the experimental Fermi surface attributable to such deviations would be obscured by broadening of the bands measured by ARPES. Therefore, the DFT calculations adopt the higher symmetry orthorhombic crystal structure with space group *Cmca* and lattice constants  $a = 5.417 \text{ \AA}$ ,  $c = 5.468 \text{ \AA}$ ,  $b = 27.962 \text{ \AA}$ , with some additional relaxation of the internal coordinates. The detailed atomic coordinates are presented in Supplementary Table 1.

**Supplementary Table 1 | The detailed atomic coordinates from the DFT calculation**

Atom	Wyckoff position	Coordinates
La1	8f	(0, 0.4326, 0.0014)
La2	8f	(0, 0.3016, 0.0099)
Ni1	4a	(0, 0, 0)
Ni2	8f	(0, 0.1394, 0.0024)
O1	8e	(0.25, 0.4921, 0.25)
O2	8f	(0, 0.0704, 0.0501)
O3	8e	(0.25, 0.3664, 0.25)
O4	8f	(0, 0.2161, 0.9641)
O5	8e	(0.25, 0.1461, 0.25)

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A comprehensive plot of the DFT results for this orthorhombic structure is shown in Supplementary Figure 4.



**Supplementary Figure 4 | DFT band structure of orthorhombic  $\text{La}_4\text{Ni}_3\text{O}_{10}$  along more directions and over a wider energy range than is shown in the main text**

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