Electronic and magnetic structure of infinite-layer NdNiO$_2$: trace of antiferromagnetic metal

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The recent discovery of Sr-doped infinite-layer nickelate NdNiO$_2$ offers a new platform for investigating unconventional superconductivity in nickelate-based compounds. Most intriguingly, the resistivity minimum and Hall coefficient drop were identified simultaneously in the experiment, reflecting a novel electronic structure and transport property of NdNiO$_2$. Driven by this pioneering work, we present a first-principles calculation for the electronic and magnetic structure of undoped parent NdNiO$_2$. By taking into account experimentally relevant interaction strength, we found that $(\pi, \pi, \pi)$ antiferromagnetic NdNiO$_2$ is a compensated bad metal with small Fermi pockets. However, due to the small exchange coupling between 3$d$-electrons of Ni and strong hybridization with 5$d$-electrons of Nd, the discovered antiferromagnetic ordering is very weak. Crucially, with the decreasing of temperature, there exists a phase transition between good paramagnetic metal and bad AFM metal. The estimated transition temperature is $\sim$70–90 K, which is consistent with that for observing the resistivity minimum and Hall coefficient drop. In this regard, our results provide a plausible physical interpretation for these significant experimental observations.

**RESULTS**

Electronic structure in PM phase

Firstly, we present the band structure of PM phase without Hubbard U. The orbital resolved band structure of PM phase is shown in Fig. 1b. Comparing with typical cuprates CaCuO$_2$, two significant differences are noted: (1) there is a gap $\sim$2.5 eV between 2$p$ orbitals of O and 3$d$ orbitals of Ni. According to Zaanan–Sawatzky–Allen classification scheme$^{15}$, this indicates that the physics of NdNiO$_2$ is close to Mott-Hubbard rather than charge-transfer$^{13,20,21}$; (2) there are two bands crossing the Fermi level, in which one is mainly contributed by $d_{x^2-y^2}$ orbital of Ni (called pure-band) and the other one has a complicated orbital compositions (called mixed-band). In $k_z = 0$ plane, the mixed-band is mainly contributed by $d_{3z^2-r^2}$ orbital of Nd and Ni. The dispersion around $\Gamma$ point is relatively small, and the pocket at $\Gamma$ point is

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called heavy electron pocket (HEP). In $k_z = 0.5$ plane, the mixed-band is mainly contributed by $d_{xy}$, $d_{xz}$, and $d_{yz}$ orbital of Nd (Ni). The dispersion around A point is relatively large, and the pocket at A point is called light electron pocket (LEP). As a comparison, one notices that there is only one pure-band crossing (Ni). The dispersion around A point is relatively large, and the pocket at A point is called light electron pocket (LEP). As a comparison, one notices that there is only one pure-band crossing the Fermi level in CaCuO$_2$\cite{13}. The Fermi surface of PM phase is shown in Fig. 1c. There is a large sheet contributed by the pure-band, as the case in CaCuO$_2$\cite{13}. This Fermi surface is obviously two-dimensional (2D), because of the weak dispersion along $\Gamma$-Z. In addition, there are two electron pockets residing at $\Gamma$ and A point, respectively, showing a feature of three-dimensional (3D) rather than 2D (see labels HEP and LEP in Fig. 1(c)). Therefore, the 3D metallic state will be hybridized with the 2D correlated state in NiO$_2$ plane, suggesting NdNiO$_2$ to be an “oxide-intermetallic” compound\cite{20,22}.

The existence of mixed-band also reflects the inherent interactions between Nd 5$d$ and Ni 3$d$ electrons. To explore the low-energy physics of NiO$_2$ superlattice, a three-band model consisting of Nd $d_{x^2−y^2}$, Nd $d_z^2$, and Nd $d_{xy}$ orbitals is constructed by Wannier90 package. As shown Fig. 1d, one can see the good agreement between first-principles and Wannier-fitting bands near the Fermi level. The little deviation between DFT and Wannier-fitting bands above the Fermi level between Z and R is due to the hybridization between Nd 5$d$ and Ni 3$d$ orbitals. Such a hybridization causes the gap open which is missing in Wannier-fitting bands. The corresponding three maximally localized WFs are shown in Fig. 1e, demonstrating the main feature of $d_{xy}$ (WF1) and $d_{xy}$ (WF2) orbital of Nd, and $d_{x^2−y^2}$ (WF3) orbital of Ni. However, these WFs still have some deviations from standard atomic orbitals, that is, WF1 and WF2 are mixed with $d_z^2$ orbital of Ni, and WF3 is mixed with $p_{xy}$ orbital of O in the NiO$_2$ plane. According to the classical Goodenough–Kanamori–Anderson rules\cite{23-25}, these deviations (or hybridizations) will give clues for the magnetic properties.

Magnetic properties

To determine the magnetic ground state of NdNiO$_2$, six collinear spin configurations are taken into account in a $2 \times 2 \times 2$ supercell, that is, AFM1 with $q = (n, n, n)$, AFM2 with $q = (n, n, 0)$, AFM3 with $q = (0, 0, n)$, AFM4 with $q = (0, 0, n)$, AFM5 with $q = (0, n, n)$, and AFM with $q = (0, 0, 0)$, as shown in Fig. 2a. Within all Hubbard U ranges, we found that AFM1 configuration always has the lowest energy, as shown in Fig. 2b, indicating a stable ($n, n, n$) AFM phase with respect to electron–electron interactions and is in accordance with random phase approximation treatment\cite{16}. This can be attributed to the special orbital distributions around the Fermi level. The intralayer NN exchange coupling is the typical 180$^\circ$ Ni–O–Ni superexchange coupling, that is, the coupling between $d_{x^2−y^2}$ orbital of Ni is mediated by $p_{xy}$ orbital of O (see WF3), preferring a ($n, n, n$) AFM phase in NiO$_2$ plane. The interlayer NN exchange coupling is due to the superexchange between the Ni $d_{x^2}$ orbitals mediated by Nd $d_{z^2}$ orbital as shown in WF1, preferring a ($n, n, n$) AFM phase between NiO$_2$ planes. Therefore, the superexchange coupling results in a stable ($n, n, n$) AFM phase in NdNiO$_2$. Moreover, the noncollinear magnetic states are further checked by including the spin-orbit coupling (SOC). We found that the spin moment prefers along $c$ direction with the magnetic anisotropic energy of $0.5$ meV/Ni. Thus, the tiny SOC effect can be safely neglected and the collinear magnetic states are used in the following phase transition temperature calculations. In cuprates, the Fermi surface is unstable with electron–electron interactions, making its parent phase to be an AFM insulator. However, this is apparently not the case in NdNiO$_2$, because of the...
extra electron pockets and the inherent interaction between Nd 5d and Ni 3d electrons. At $U = 0$ eV, there are two electron pockets at $\Gamma$ point and two hole pockets along X–R direction as shown in Fig. 3a, b. Physically, the origin of these four pockets can be easily understood through the comparison of orbital resolved band structures between PM phase (Fig. 1b) and ($\pi$, $\pi$, $\pi$) AFM phase (Fig. 4). Because of the Zeeman field on Ni, its spin-up and spin-down bands are split away from each other. The original pure-band ($d_{x^2-y^2}$ orbital of Ni) in PM phase becomes partially occupied in spin-up channel (forming two hole pockets) and totally unoccupied in spin-down channel. Hence, the two hole pockets in AFM phase are inherited from large sheet in PM phase, showing a 2D character with negligible dispersion along $\Gamma$–Z direction. For the electron pockets at $\Gamma$ point, the heavier one is mainly contributed by Ni, so it comes from the HEP at $\Gamma$ point of PM phase. While for the lighter one, it comes from the LEP at A point of PM phase which is folded into the $\Gamma$ point of ($\pi$, $\pi$, $\pi$) AFM phase [see Fig. 1a].

These pockets have a different evolution with the increasing value of Hubbard $U$. For electron pockets, the heavier one is very sensitive to Hubbard $U$ and disappears at $U = 1$ eV. Meanwhile the lighter one does not disappear until $U = 6$ eV. In addition, the
orbital components of lighter electron pockets are purified by electron–electron interaction and it is mainly contributed by d_{xy} of Nd in the large U limit as shown in Fig. 4. The case for hole pockets is rather complicated. Firstly, the bands of hole pockets become flat with the increasing value of Hubbard U. Secondly, the original hole pockets formed by d_{x^2-y^2} orbital of Ni gradually disappear, meanwhile, a new hole pocket formed by d_{z^2} orbital of Ni appears along Γ–M as shown in Fig. 3d. At U = 6 eV, NdNiO$_2$ is a compensated metal with a small electron pocket at Γ point and four hole pockets along Γ–M as displayed in Fig. 3e. Further increasing the value of Hubbard U, the gap between 3d orbital of Ni and 2p orbital of O gradually decreases (Fig. 4), demonstrating an evolution from Mott-Hubbard metal to charge-transfer insulator.

For the magnetic ground state, so far, no consensus has been reached. For example, most of studies assumed the (\(\pi, \pi, 0\)) AFM order as the ground state, without a detailed energetic investigation, e.g. Gu et al., Botana et al., and Lee et al. Additionally, Zhang et al. and Hepting et al. calculated band structures based on (\(\pi, \pi, 0\)) AFM order. Most importantly, the detailed analysis of magnetic ground state is missing in all previous works. In this work, we compare a large number of magnetic configurations and found (\(\pi, \pi, m\)) (rather than (\(\pi, \pi, 0\))) to be the magnetic ground state.

We speculate that this orbital switching may change the paradigm after doping. Moreover, without the Hubbard U, the 2p orbital of O is far away from the Fermi level, just like the case of PM phase. However, with the increasing value of Hubbard U, the gap between 3d orbital of Ni and 2p orbital of O gradually decreases (Fig. 4), demonstrating an evolution from Mott-Hubbard metal to charge-transfer insulator.

Fig. 4 Orbital resolved band structures of (\(\pi, \pi, m\)) AFM phase with different values of Hubbard-U. The first, second, third, and forth row represents Nd, spin-up Ni, spin-down Ni, and O, respectively. The filled circles with different colors have the same meaning as those in Fig. 1. The name of d orbitals in the AFM supercell has been aligned to that of unit cell.
PM-AFM transition

In order to quantitatively describe such a phenomenon, the phase transition temperature is further calculated. For \((n, n, n)\) AFM phase, the magnetic momentum of Ni increases from 0.58 \(\mu_B\) at \(U = 0\) eV to 1.04 \(\mu_B\) at \(U = 8\) eV and becomes gradually saturated, as shown in Fig. 5a. This is also consistent with the fact that \(d_{x^2-y^2}\) orbital of Ni is closer to single occupation with the increasing value of Hubbard \(U\). Therefore, Ni is spin one half \((S = 1/2)\) in infinite-layer NdNiO2, just like the case in cuprates. To extract the exchange coupling parameters of \(J_1, J_2, J_3,\) and \(J_4\) (as labeled in Fig. 2a), the total energy of five AFM configurations obtained from DFT + U calculations are mapped onto the Heisenberg spin Hamiltonian. In the \(2 \times 2 \times 2\) supercell, there are 8 Ni atoms and the total energy of different AFM configurations are:

\[
\begin{align*}
E_{AFM1} &= E_0 - 16J_1S^2 - 8J_2S^2 + 16J_3S^2 + 32JS^2 \\
E_{AFM2} &= E_0 - 16J_1S^2 + 8J_2S^2 + 16J_3S^2 - 32JS^2 \\
E_{AFM3} &= E_0 + 16J_1S^2 - 8J_2S^2 + 16J_3S^2 - 32JS^2 \\
E_{AFM4} &= E_0 + 8J_2S^2 - 16J_3S^2 + 32JS^2 \\
E_{AFM5} &= E_0 - 8J_2S^2 - 16J_3S^2 - 32JS^2
\end{align*}
\]

(1)

where \(E_0\) is the reference energy without magnetic order. Only \((n, n, n)\) and \((n, n, 0)\) are stable at \(U = 0\) eV, and we ignore results at \(U = 0\) eV in the following discussions. The calculated exchange coupling parameters as a function of Hubbard \(U\) are shown in Fig. 5b. We would like to make several remarks here: (1) the NN intralayer exchange coupling \(J_1\), mediated by \(d_{x^2-y^2}\) orbital of Ni, demonstrates a \(1/U\) law; (2) the NN interlayer exchange coupling \(J_2\) is \(\sim 10\) meV with little variation. The positive value of \(J_2\) indicates an AFM coupling between NiO2 planes; (3) the next NN interlayer exchange coupling \(J_3\), mediated by \(d_{xy}\) orbital of Nd, is comparable to \(J_1\) at large value of Hubbard \(U\), which is dramatically different to that in infinite-layer SrFeO2; (4) the next NN interlayer exchange coupling \(J_4\) is \(\sim 0\) meV, indicating the validity of our Hamiltonian up to the third NN; (5) \(J_1, J_2,\) and \(J_3\) have the same strength at large \(U\), suggesting NdNiO2 is a 3D magnet rather than 2D magnet.

Based on the above exchange coupling parameters, the phase transition temperature \(T_{N}\) is calculated by classical Monte Carlo method in a \(12 \times 12 \times 12\) supercell based on the classical spin Hamiltonian:

\[
H = \sum_{\langle i,j \rangle} J_{ij} S_i \cdot S_j
\]

(2)

where the spin exchange parameters \(J_{ij}\) have been defined above.

First, we calculate the specific heat \(C\) after the system reaches equilibrium at a each given temperature \(T\), as shown in Fig. 5c. Then, \(C\) is extracted from the peak position in the curve of \(C(T)\), as shown in Fig. 5c. For \(U = 1\) eV, \(T_N\) is as high as 220 K, which can be ascribed to the large value of \(J_1\). With the increasing value of Hubbard \(U\), \(T_N\) gradually decreases and becomes \(\sim 70\) K at \(U = 6\) eV. To further check the effect of interlayer exchange coupling on 3D magnet, an additional Monte Carlo calculation is performed without \(J_2\) and \(J_4\). As shown in Fig. 5e, the \(C(T)\) vs \(C(T)\) plot shows a broaden peak at a lower temperature. Since Mermin-Wagner theorem prohibit magnetic order in 2D isotropic Heisenberg model at any nonzero temperatures, the broad peak in \(C(T)\) vs \(T\) plot implies the presence of short-range order. Regarding the small drop of \(T_N\) (\(\sim 30\) K in Fig. 5f), our MC simulations indicate that the weak interactions between NiO2 planes.

Experimental relevance

To address the relevance of the current calculations and experimental observations, we first estimate the value of Hubbard interaction strength \(U\). Although the exact value of Hubbard \(U\) cannot be directly extracted from the first-principles calculations, its value range can still be estimated based on similar compounds. The infinite-layer nickelate is believed to be a worse metal compared to elemental nickel with \(U \sim 3\) eV36, which can be considered as a lower bound of Hubbard \(U\). The Coulomb interaction in infinite-layer nickelates should be smaller than that in the charge-transfer insulator NiO with \(U \sim 8\) eV37, which can be considered as a upper bound of Hubbard \(U\). Therefore, a reasonable value of Hubbard \(U\) in NdNiO2 will be between 3 eV and 8 eV. In the following discussion, we would like to use the median value, \(U \sim 5-6\) eV.

Fig. 5  Dependence of magnetic properties on Hubbard \(U\). The Hubbard \(U\) dependence of a the magnetic momentum of Ni in \((n, n, n)\) AFM phase, b the exchange coupling parameters, c specific heat \((C)\) vs \(T\) with four \(J_i\), d the estimated \(T_N\) with four \(J_i\), e specific heat \((C)\) vs \(T\) with \(J_1, J_2,\) and \(J_3\) only and f the estimated \(T_N\) with \(J_1, J_2,\) and \(J_3\) only. The shaded region in d highlights the possible \(T_N\) of 70–90 K with a reasonable \(U \sim 5-6\) eV.
Second, if the interaction strength is around \( U \sim 5-6 \text{ eV} \), the estimated magnetic exchange interaction is around \( J_1 \sim 10 \text{ meV}, J_2 \sim 10 \text{ meV}, J_3 \sim 13 \text{ meV} \) (see Fig. 5b). This indicates that, effective exchange interactions in NdNiO\(_2\) are about one-order smaller than those of cuprates \( \sim 112 \text{ meV}^{21,38-44} \). Also it results in a relative weaker magnetic ordering and lower Neel temperature \( T_N \) in NdNiO\(_2\) compared with cuprates (see below).

Third, to further discuss the magnetic transition temperature, we show the Neel temperature dependence on interaction strength in Fig. 5d. Within the estimated interaction range \( U \sim 5-6 \text{ eV} \), we find the Neel temperature, which separates the PM phase from the \((n, \pi, \pi)\) AFM phase, is near \( 70-90 \text{ K} \). Interestingly, this coincides with the minimum in resistivity and the drop in Hall coefficient\(^6\). It provides a novel understanding of minimum in resistivity, i.e. partial electrons tend to localize and form magnetic order, therefore the conducting carriers decreases. Thus, our calculation indicates that, the resistivity minimum and the drop in Hall coefficient relates to the magnetic phase transition at the Neel temperature.

Fourth, previous power neutron scattering measurement on NdNiO\(_2\) did not find the signal of AFM ordering\(^{45,46}\). This could be attributed to the following reason. The estimation of Neel temperature (in Fig. 5d) does not include the influence of conduction electrons. We notice that, there are small Nd 5d-electron pockets near the Fermi surface at the critical interaction strength (Fig. 3e). By concluding the hybridization effect between Nd 5d-electrons and Ni 3d-electrons, there are at least two influences. On one hand, it is expected that the local magnetic AFM ordering below the Neel temperature is further weakened. On the other hand, the magnetic phase transition is replaced by a crossover from normal metal to bad AFM metal around \( T_N \sim 70-90 \text{ K} \), which is more likely to occur in the experiment\(^6\). Both of the above effects lead to further weaken the AFM ordering\(^{26,46}\), which could be hard to detect in neutron scattering measurement.

Lastly, some recent experiments fail to find bulk superconductivity in NdNiO\(_2\) systems, and the parent samples show strong insulating behaviors\(^7\). The insulating behavior could be attributed to strong inhomogenous disorder or improper introduction of H during the reaction with \( \text{CaH}_2\).\(^{48}\) Especially, it is worth noting, these experiments cannot rule out the possibility of weak AFM ordering, due to the presence of Ni impurities in their samples. (Actually this problem has been pointed out before\(^{35,46}\).) The strong ferromagnetic order from elemental Ni would dominate over and wash out the weak signal of AFM ordering from NdNiO\(_2\) as we suggested in this work.

Taken as a whole, we conclude that, our calculations provide a self-consistent understanding on the experimental observation\(^6\), the resistivity minimum and drop in Hall coefficient is related to the crossover from normal metal to bad AFM metal around \( T_N \sim 70-90 \text{ K} \). The AFM ordering at lower temperature is weak due to the hybridization or self-doping effect, which is hard to detect in the previous measurements. In this regarding, the upcoming inelastic neutron scattering on high-quality samples is highly desired.

**DISCUSSION**

In this work, we present a systematic study of the electronic and magnetic properties of parent compound NdNiO\(_2\) by first-principles calculations combined with classical Monte Carlo calculations. The Fermi surface of PM phase is quite large with two 3D-like electron pockets, which is consistent with the previous work\(^{13-16,18}\). By tuning the interaction strength, before it enters correlated insulator, NdNiO\(_2\) is a compensated metal with one small electron pocket formed by \( d_{x^2} \) orbital of Nd and four small hole pockets formed by \( d_{x^2} \) orbital of Ni. We identify the interaction selects a \((n, \pi, \pi)\) AFM order as the correct magnetic ground state. In the reasonable estimation \( U = 5-6 \text{ eV}^{20,37} \), we find several conclusions related to the experiment\(^6\): (1) the exchange-coupling parameters are \( -10 \text{ meV} \), which is one order smaller than cuprates\(^{21,38-44}\) and results in a low \( T_N \) compared with cuprates; (2) the self-doing effect from 5d orbital of Nd and 3d orbital of Ni may screen the local magnetic momentum in \( d_{x^2} \) orbital of Ni, which gives a small magnetic momentum less than \( 1 \mu_B \) and makes the long-range AFM order unstable\(^{65,49,46}\); (3) with the decreasing of temperature, there is a phase transition from PM phase to \( (n, \pi, \pi) \) AFM phase near \( 70-90 \text{ K} \). Therefore, there could exist a transition from normal metal to bad AFM metal around \( T_N \sim 70-90 \text{ K} \), which provides a plausible understanding of minimum of resistivity and Hall coefficient drop in infinite-layer NdNiO\(_2\). We envision that our calculations will intrigue intensive interests for studying the magnetic properties of high-quality infinite-layer NdNiO\(_2\) samples.

**METHODS**

The first-principles calculations are carried out with the plane wave projector augmented wave method as implemented in the Vienna ab initio simulations package (VASP)\(^{50-52}\). The Perdew–Burke–Ernzerhof (PBE) functionals of generalized gradient approximation (GGA) is used for PM phase\(^53\). To incorporate the electron-electron interactions, DFT + \( U \) is used for AFM phase, which can reproduce correctly the gross features of correlated-electrons in transition metal oxides\(^{54-56}\). There are two kinds of strongly localized orbitals in NdNiO\(_2\): 4f of Nd and 3d of Ni. The 4f electrons of Nd are expected to display the local magnetic moment as Nd\(^{3+}\) in Nd\(_2\)CuO\(_4\).\(^57\) The hybridization between \( f \) electrons and superconducting plane is very complicated. In Eu\(_2\)Fe\(_2\)As\(_2\), superconductivity in FeAs layers and ferromagnetism in Eu layers can coexist. In PrBa\(_2\)Cu\(_4\)O\(_y\), where the local environment of the 4f ion is the same as in NdNiO\(_2\), the antibonding coupling of the Pr\(_{f_{22}}\) orbital to the O 2p orbitals makes PrBa\(_2\)Cu\(_4\)O\(_y\) not superconducting\(^58\). Recently, it has been proposed that the intra-atomic 4f-5d exchange coupling of Nd may change the understanding of the superconducting properties in NdNiO\(_2\).\(^59\) Since the local magnetic moment of Nd\(^{3+}\) is weakly coupled in NdNiO\(_2\), here we ignore the possibility of local moment formed by 4f electron of Nd\(^{3+}\) in our calculation by treating them as the core-level electrons and focus only on the magnetic order fromed by Ni. The Hubbard \( U (0-8 \text{ eV}) \) term is added to 3d electrons of Ni. The energy cutoff of 600 eV, and Monkhorst-Pack \( k \) point mesh of \( 11 \times 11 \times 11 \) and \( 18 \times 18 \times 30 \) is used for PM and AFM phase, respectively. The maximally localized Wannier functions (WFs) are constructed by using Wannier90 package\(^{61,62}\). The structure of infinite-layer NdNiO\(_2\) is shown in Fig. 1a, including O\(_2\) layers sandwiched by Nd, which can be obtained from the perovskite NdNiO\(_2\) with reduction of apical O atoms in c direction\(^56,60\). Due to apical O vacancies, the lattice constant in \( c \) direction shrinks (smaller than \( a \) direction) and the space group becomes \( P4/mmm \). The experimental lattice constant \( a/b = 3.92 \text{ Å} \) and \( c = 3.28 \text{ Å} \) are used in our calculations.

**DATA AVAILABILITY**

The numerical datasets used in the analysis in this study, and in the figures of this work, are available from the corresponding author on reasonable request.

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COMPETING INTERESTS
The authors declare no competing interests.

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