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ABSTRACT

The observation of superconductivity in infinite-layer nickelates provides an appealing new platform to explore a superconducting mechanism. Rationalizing the ground state magnetic order and spin dynamics in undoped compounds are the foundation for understanding the superconducting mechanism. Here, magnetic properties of infinite-layer $LaNiO_2$ are investigated and compared with cuprate analog $CaCuO_2$ by combining first-principles and spin-wave theory calculations. We reveal that $LaNiO_2$ exhibits quasi-two-dimensional (2D) antiferromagnetic (AFM) order that mimics that of cuprate superconductors. Moreover, the electronic origin of the quasi-2D AFM state and the simulated dispersion of magnetic excitations in $LaNiO_2$ show strong resemblance to that of $NdNiO_2$. The establishment of a direct connection with the cuprates from the electron, orbital, and spin degrees of freedom provides solid theoretical basis to elucidate the origin of superconductivity in infinite-layer nickelates.

Infinite-layer nickelates $RNiO_2$ are currently attracting intense research interest owing to the discovery of superconductivity with hole doping.[1] These intriguing observations have reinvigorated theoretical and experimental explorations of the puzzling mechanism behind the high-temperature superconductor.[1–49] Antiferromagnetic (AFM) spin fluctuations have long been considered as a possible mechanism for the appearance of unconventional superconductivity.[50–52] A recent experiment based on resonant inelastic x-ray scattering (RIXS) has confirmed the quasi-two-dimensional (2D) AFM state in $NdNiO_2$, and the exchange constants are extracted by a linear spin wave theory.[4] However, the presence and nature of magnetic interactions in $LaNiO_2$ is still under debate.

Both a paramagnetic ground state[45] and an intrinsic magnetic ground state[32,46] are proposed in recent experiments. On the theoretical side, $LaNiO_2$ was initially reported as an insulating and AFM system by Anisimov *et al.*[53] Subsequent study by Lee and Pickett reported a metallic and AFM ground state.[54] Soon after the discovery of superconductivity in infinite-layer nickelates,[1] the electronic and magnetic properties of $LaNiO_2$ have recently been intensively studied by first-principles calculations. However, both C-type AFM (C-AFM)[12–14] and G-type AFM (A-AFM)[14–16] ground states are proposed by different works, relying on the employed functional and Hubbard U. The similar superconducting phase diagram in hole-doped isoelectronic and isostructural $LaNiO_2$ (Ref. 47) and $NdNiO_2$ (Refs. 7 and 8) indicates that they may have a general superconducting mechanism. Therefore, it is highly desirable to identify the magnetic ground state of $LaNiO_2$, which is not only of scientific interest but also of critical importance for disentangling the key factor responsible for the superconductivity.

In this work, the electronic and magnetic properties of $LaNiO_2$ are theoretically investigated by a comparative study with $CaCuO_2$. Despite the metallic nature of $LaNiO_2$, our results suggest the presence of quasi-2D AFM order, similar with insulating $CaCuO_2$. Additionally, the magnetic excitation dispersion is comparable with $NdNiO_2$, implying that the magnetic interaction may be an intrinsic property of $RNiO_2$ compounds. The electronic origin of the quasi-2D AFM order is rationalized by the analysis of orbitals contributed exchange constants. Our work, thus, provides an important complementary for the knowledge of magnetic properties in the appealing $RNiO_2$ system and highlights that AFM interactions that are critical in cuprate superconductors may also play a non-negligible role in the superconducting property of doped $LaNiO_2$.

The ground state properties of $LaNiO_2$ are investigated by the density-functional theory (DFT) plus U[55] method as implemented in the Vienna *ab initio* simulation package (VASP).[72,73] Both the Perdew–Burke–Ernzerhof (PBE)[56] and Perdew–Burke–Ernzerhof

exchange-correlation functional revised for solid (PBEsol)[57] functionals were employed in the calculations. The rev-vdW-DF2[58] and vdW-DF-cx[59] functionals are also used for the structural property to examine the effect of the dispersion forces. A plane-wave energy cutoff of 700 eV and a $9 \times 9 \times 7$ Monkhorst-Pack k-point mesh[60] were used for the $\sqrt{2} \times \sqrt{2} \times 2$ supercells. During the geometry optimizations, the atomic positions and lattice constants are fully relaxed until the energy and Hellmann–Feynman force convergence of 10^{-7} eV and 10^{-3} eV/Å is achieved. Phonon frequencies were derived from the PHONOPY code[61] using the finite displacement approach. The exchange constants were estimated from the TB2J code[62] with the results from maximally localized Wannier functions.[63,64] The magnetic excitation spectra were computed by the SpinW code[65] with the exchange constants derived from TB2J.

We first focus on the effect of Hubbard U[55] on the ground state properties. Here, U values ranging from 0 to 5 eV are selected in the PBE + U and PBEsol + U methods. Full optimizations of the lattice constants and atomic positions in the $P4/mmm$ phase and the low-symmetry $I4/mcm$ phase (recently considered as the ground state of the RNiO$_2$ system with smaller R-site cations[29,48,49]) with ferromagnetic (FM), A-type AFM (A-AFM), C-AFM, and G-AFM states are performed to theoretically determine the lowest-energy magnetic state and structure. Figures 1(a) and 1(b) present the energy difference between different phases. For the PBEsol + U method, we can see that the G-AFM $P4/mmm$ phase always has the lowest energy when U = 0–3 eV, and the energies of G-AFM and C-AFM become almost the same for U = 4 and 5 eV. However, we also see that the U value in the PBE + U method has strong effect on the magnetic and structural ground state. When U is equal or smaller than 2 eV, the G-AFM $P4/mmm$ phase is the ground state; however, the low-symmetry $I4/mcm$ phase with the C-AFM state has the lowest energy when U is larger than 2 eV in line with previous work.[14] The structural instability is further supported by the U value dependent phonon frequency of rotation motion shown in Figs. 1(c) and 1(d). It is obvious that the phonon frequency gradually decreases with the increase in the U value, and the imaginary frequency appears for PBE + U with U = 3–5 eV. As there is no experimental evidence for rotation motion and temperature dependent resistivity anomaly as observed in NdNiO$_2$,[1] it can be concluded that PBE + U with U larger than 2 eV could not give the proper ground state structure for LaNiO$_2$.

The variations in the phonon frequency of rotation motion from rev-vdW-DF2 + U and vdW-DF-cx + U are plotted in Figs. S1(a) and S1(b), respectively. Obviously, increasing the U value of the vdW-DF-cx functional similarly softens the rotation motion as the PBE + U method. Figure S2 compares the phonon dispersions from four different functionals with different U values, and it is apparent that the phonon dispersions have similar characteristics and frequencies expected for the A_4^- mode. The A_4^- rotation mode is very sensitive to the Hubbard U value, and increasing the U value could similarly enhance the instability of rotation. The lattice constants from different functionals with different U values are compared in Fig. S3. It is evident that the predicted lattice constants all are very close to the experimental values.[66] Among them, the PBE and PBE + U provide more accurate lattice constants compared with the other functionals. Therefore, the dispersion component seems to have small effects on the lattice constants, atomic position, and phonon dispersions, and all the four functionals (PBE, PBEsol, rev-vdW-DF2, and vdW-DF-cx) with reasonable U values can naturally describe the layered systems.

It is worth mentioning that our results from strongly constrained and appropriately normed (SCAN) functional[67] support the C-AFM magnetic ground state consistent with previous works.[13] Although the properties of insulating cuprate, such as La$_2$CuO$_4$, are well reproduced by the SCAN functional,[68] the SCAN functional is demonstrated to overestimate the magnetization and magnetic energy of metals.[69] As shown in Fig. S4 of the supplementary material, the SCAN functional strongly overestimates the spin splitting of metallic $d_{3z^2-r^2}$ bands compared with PBE (sol) + U methods, which could give unreasonable interlayer FM coupling according to our discussion in the following.

Next, we focus on the exchange constants of G-AFM $P4/mmm$ LaNiO$_2$ to determine the magnetic dimensionality. Figure 2(a) shows

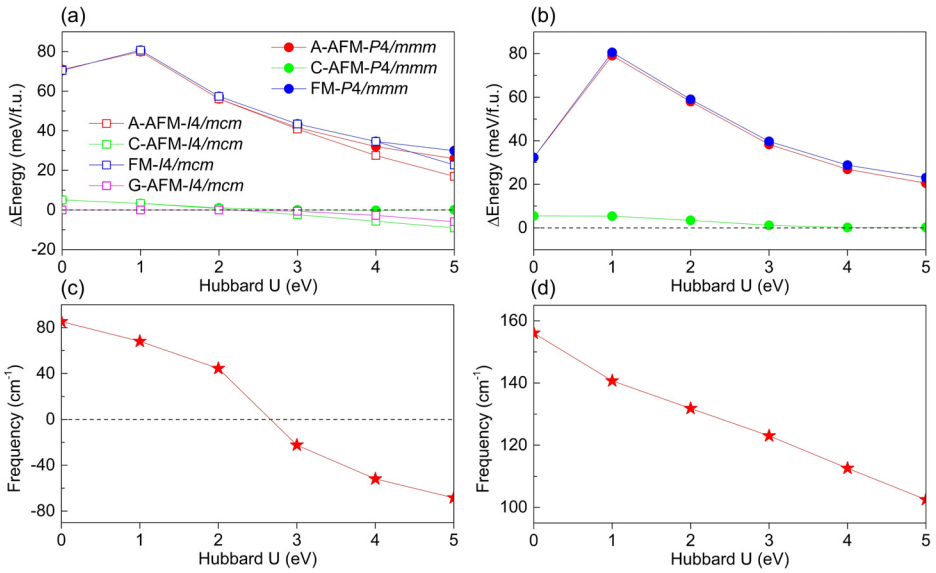

FIG. 1. Hubbard U dependence of ground state properties. Energy difference of the A-type AFM (A-AFM) $P4/mmm$ phase, the C-AFM $P4/mmm$ phase, the FM $P4/mmm$ phase, the A-AFM $I4/mcm$ phase, the C-AFM $I4/mcm$ phase, the FM $I4/mcm$ phase, and the G-AFM $I4/mcm$ phase with respective the reference G-AFM $P4/mmm$ phase for LaNiO$_2$ as a function of the U value for (a) PBE functional and (b) PBEsol functional. Phonon frequency of in-plane rotation motion (A_4^-) as a function of the U value for (c) PBE functional and (d) PBEsol functional.

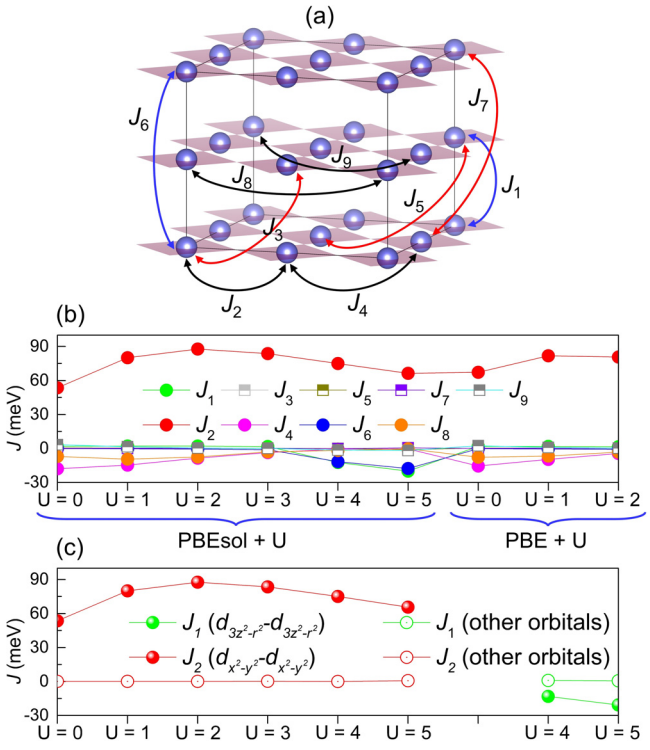

FIG. 2. (a) Schematic representation of nine exchange interactions in $LaNiO_2$. (b) The amplitude of nine exchange constants for PBEsol + U and PBE +U methods with different U values. (c) The orbital contributions of first-neighbor exchange constants from PBEsol + U.

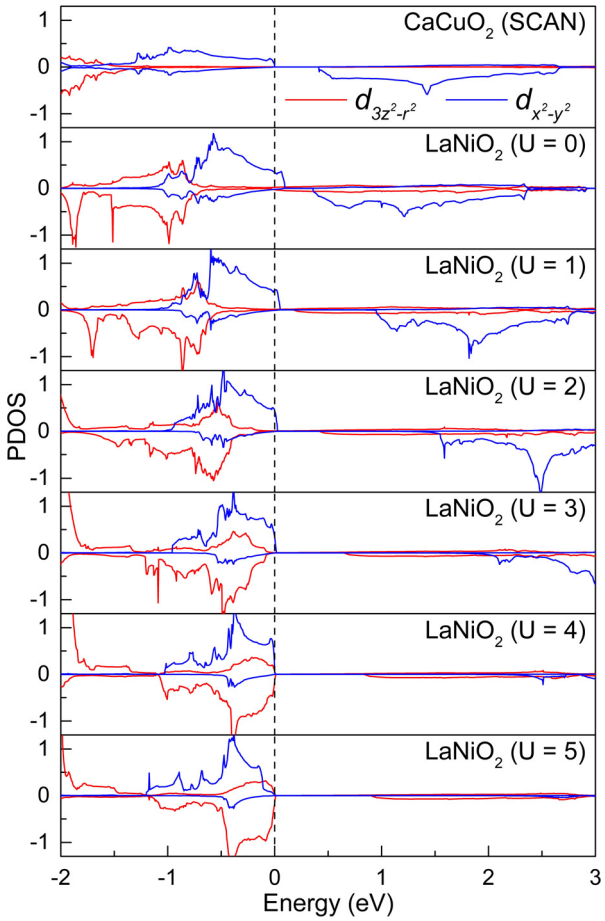

FIG. 3. The PDOS of $CaCuO_2$ from the SCAN functional and $LaNiO_2$ from PBEsol + U with different U values.

the schematic picture of nine nonequivalent Heisenberg couplings considered here. The Hubbard U dependent exchange constants estimated from the TB2J code[62] are plotted in Fig. 2(b). For relatively small U values ($U \leq 3$ eV), it is found that three in-plane exchange constants J_2, J_4, and J_8 are the dominant, while the other out-of-plane exchange constants are rather weaker compared to in-plane exchange constants. The first-neighbor in-plane exchange constant is around 50 times of first-neighbor out-of-plane exchange constant, indicating a quasi-2D AFM state. Regarding larger U values ($U = 4$ and 5 eV) in PBEsol + U, we see that the out-of-plane FM interactions J_1 and J_6 become non-negligible, and this gives rise to a three-dimensional (3D) magnetic characteristic.

To clarify the effect of Hubbard U on the out-of-plane FM interactions, we give further insight into the electronic structure of $LaNiO_2$ with the PBEsol + U method and $CaCuO_2$ with the SCAN functional in Fig. 3. In terms of small U values ($U \leq 3$ eV), the $d_{3z^2-r^2}$ bands are nearly fully occupied below the Fermi level, and the $d_{x^2-y^2}$ bands are almost half occupied and dominate the states around the Fermi level, which is also similar to $CaCuO_2$. With an increase in the U value, we see that the band edge of the $d_{3z^2-r^2}$ band gradually increases and even goes across the Fermi level for $U = 4$ and 5 eV in agreement with previous works.[14,54] Figure 2(c) compared the first-neighbor in-plane and out-of-plane exchange constants and their orbital contributions for $LaNiO_2$. Obviously, the coupling between $d_{x^2-y^2}$ orbitals is the primary source of the in-plane exchange constants. As the couplings between spin polarized $d_{3z^2-r^2}$ electrons would lead to out-of-plane FM interactions, the Hubbard U controlled Fermi surface is likely responsible for stabilizing the 3D magnetic dimensionality for $U = 4$ and 5 eV.

To disentangle the direct effect of the out-of-plane FM interaction on the magnetic excitations, the spin-wave dispersions of $LaNiO_2$ and $NdNiO_2$ from PBEsol + U ($U = 4$ and 5 eV) are examined as shown in Fig. S5 of the supplementary material. It is observed that all the spectra exhibit notable dispersion along the out-of-plane (0.25, 0, 0)–(0.25, 0, 0.5) path, in apparently contrast to the RIXS results of $NdNiO_2$,[4] where there is unnoticeable dispersion along the (0.25, 0, 0.25)–(0.25, 0, 0.39) path. Hence, it is obvious that larger Hubbard U values significantly overestimate the out-of-plane FM couplings and cannot give a reliable magnetic excitation spectrum, which will be eliminated.

It is known that the Hubbard U parameter can be fitted by constrained random phase approximation (cRPA) calculations[70] and the linear response method.[71] We note that the recent cRPA calculations suggest a range of U values from 2.1–6.8 eV dependent on the selected orbitals in $NdNiO_2$.[28] We also made a careful reexamination of the fitted Hubbard U with the linear response method. It is found that the

fitted U values are 6.3 and 6.4 eV for PBE and PBEsol functionals (see Fig. S6).[72] From the evolution of the phonon frequency shown in Fig. 1 and the above discussions, it is obvious that such larger U values would overestimate the instability of rotation motion and result in the low-symmetry $I4/mcm$ phase for the PBE functional, inconsistent with the experiments.[66] For the PBEsol functional, much larger and unreasonable out-of-plane exchange constants and magnetic dispersion along the out-of-plane direction would be obtained with such a larger U value according to Fig. 2(a) and Fig. S5. We may, therefore, conclude that $LaNiO_2$ with suitable Hubbard U values exhibits a quasi-2D Neel-type AFM ground state similar to $CaCuO_2$.

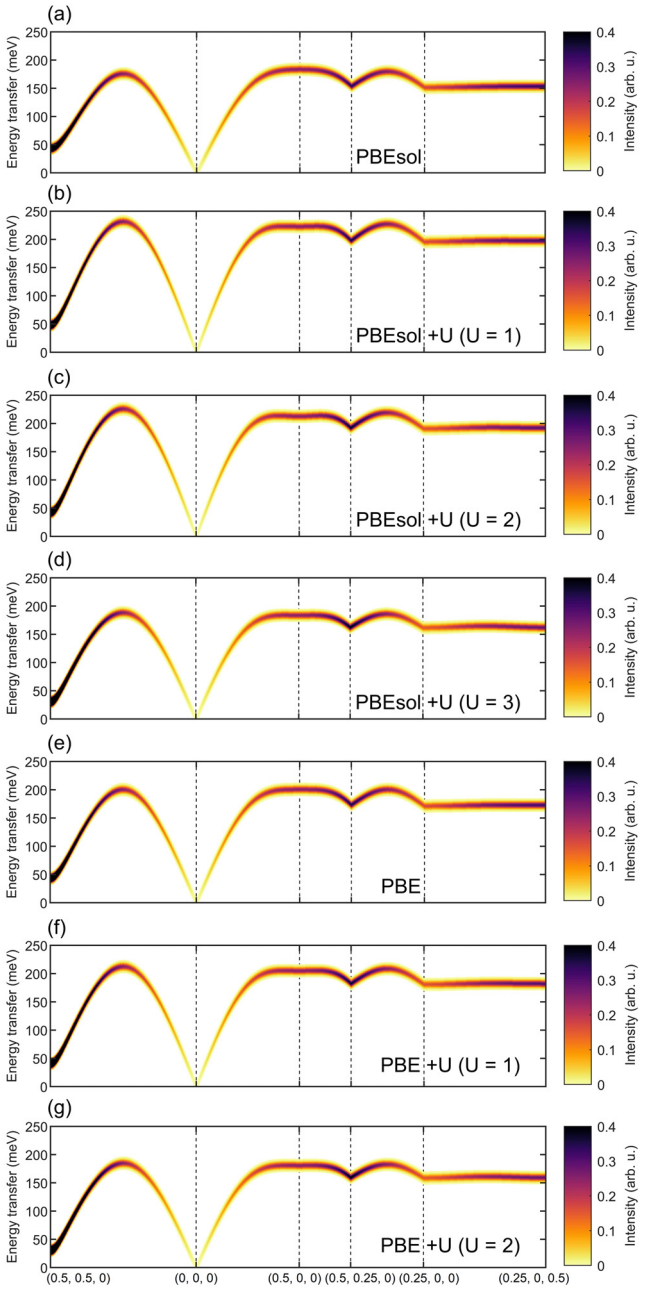

FIG. 4. The spin-wave dispersions of $LaNiO_2$ obtained from (a) the PBEsol functional, (b) PBEsol + U (U = 1 eV), (c) PBEsol + U (U = 2 eV), (d) PBEsol + U (U = 3 eV), (e) the PBE functional, (f) PBE + U (U = 1 eV), and (g) PBE + U (U = 2 eV).

Finally, to further inspire experimental work to verify the predicted 2D magnetic interactions in $LaNiO_2$, spin-wave spectra, which could be measured in experiments, are calculated with eight dominant exchange constants. Figure 4 illustrates the predicted spin-wave spectra based on the linear spin-wave theory with PBE + U and PBEsol + U. Interestingly, the spin-wave spectra closely resemble the features previously found in $NdNiO_2$:[4] (i) the low-energy branch emerges from the Brillouin zone center point (0, 0) and reaches up the maximum at (0.5, 0) and (0.25, 0.25); (ii) the dispersive bandwidth of around 173–233 meV dependent on the functional and Hubbard U is comparable with $NdNiO_2$; (iii) there is strong intensity near (0.25, 0.25), while a relative weak intensity at another maxima of (0.5, 0). Given the similarity in the spin-wave spectra with $NdNiO_2$, our results further strengthen our statement that there are robust magnetic interactions in $LaNiO_2$, and it behaves as a spin-1/2 square-lattice Heisenberg AFM system.

In summary, by investigating the structural, electronic, and magnetic properties of $LaNiO_2$, we predict that $LaNiO_2$ is a 2D AFM material with $d_{x^2-y^2}$ orbitals occupying the Fermi surface, analogous to $CaCuO_2$. We further give detailed insight into the essential influence of Hubbard U on the lattice instability, crystal splitting, and exchange interactions and have found suitable U values to give reasonable description of properties related to the experimental results. The results indicate that increasing the U value acts to increase the band edge and spin splitting of the $d_{3z^2-r^2}$ bands. Direct connections between Hubbard U-Fermi surface-magnetic dimensionalities are established, which could reconcile contradictory predictions on the magnetic dimensionality (2D or 3D). More importantly, the predicted magnetic excitation spectrum of $LaNiO_2$ displays remarkably $NdNiO_2$-like characteristics, and this finding provides vivid theoretical support for the recent demonstration of the intrinsic magnetic ground state of $RNiO_2$, regardless of the rare earth ion.

See the supplementary material for the phonon frequency from vdW-DF-cx + U and rev-vdW-DF2 + U, phonon dispersions, lattice constants, PDOS from different functional and Hubbard U, the spin-wave dispersions of $LaNiO_2$ and $NdNiO_2$ from PBEsol + U (U = 4 and 5 eV), and the data for fitting U from the linear response method.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Yajun Zhang: Conceptualization (lead); Data curation (lead); Formal analysis (lead); Funding acquisition (lead); Investigation (lead); Methodology (lead); Project administration (lead); Resources (lead); Software (lead); Supervision (lead); Validation (lead); Visualization (lead); Writing – original draft (lead); Writing – review & editing (lead). **Xu He:** Formal analysis (supporting); Methodology (supporting); Writing – review & editing (equal). **Philippe Ghosez:** Formal analysis (supporting); Supervision (equal); Writing – review & editing (supporting).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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