

Heterostructuring as Gateway to Electron Doping of Nickelate Superconductors

Chao Deng¹, Motoharu Kitatani^{2,3}, Guiwen Jiang⁴, Siqi Guo¹, Niklas Witt⁵, Ao Zhang^{1,6}, Wenfeng Wu^{7,8,9}Mi Jiang⁴, Karsten Held⁹, and Liang Si^{1,10,11,9,*}¹*School of Physics, Northwest University, Xi'an 710127, China*²*Department of Material Science, University of Hyogo, Ako, Hyogo 678-1297, Japan*³*Graduate School of Engineering, Kyushu Institute of Technology, Kitakyushu 804-8550, Japan*⁴*School of Physical Science and Technology, Soochow University, Suzhou 215006, China*⁵*Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ctd.qmat, Universität Würzburg, 97074 Würzburg, Germany*⁶*Department of Physics, Southeast University, Nanjing 211189, China*⁷*Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences, Hefei 230031, China*⁸*Science Island Branch of Graduate School, University of Science and Technology of China, Hefei 230026, China*⁹*Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria*¹⁰*Shaanxi Key Laboratory for Theoretical Physics Frontiers, Xi'an 710127, China*¹¹*Fundamental Discipline Research Center for Quantum Science and technology of Shaanxi Province, Xi'an 710127, China*

(Received 26 January 2026; accepted 23 June 2026; published 20 August 2026)

Despite enormous expenditures in the research field, the electron-doped side of nickelate superconductors remains uncharted territory. Substituting the trivalent rare-earth cations by a tetravalent one hitherto failed. Here, we demonstrate by first-principles calculations a disorder-free route to electron dope Ruddlesden-Popper nickelates. When intercalating wide-band-gap insulating layers such as LaXO_3 ($X = \text{Al, Ga, Sc}$) into La_2NiO_4 , the extra $(\text{LaO})^+$ layers act as electron donors, releasing carriers into the $\text{Ni-}3d$ orbitals. This electron doping puts $\text{La}_2\text{NiO}_4:\text{La}_2\text{AlO}_4$ naturally in the optimal region for $d_{x^2-y^2}$ -wave superconductivity with T_c exceeding 50 K. The same concept also allows us to electron dope $\text{La}_3\text{Ni}_2\text{O}_7$, the superconductor in the limelight.

DOI: 10.1103/qp4p-x6g3

Introduction—A central motif for unconventional superconductors such as cuprates [1–4] and nickelates [5–9] is doping. This doping is required to suppress the antiferromagnetic insulating state of the parent compound with superconductivity emerging in a narrow window of doping next to this antiferromagnetic ordering. In cuprates such as La_2CuO_4 [1,10], superconductivity emerges upon hole doping via alkaline-earth substitution such as replacing La^{3+} by Sr^{2+} or Ca^{2+} . This drives the Cu^{2+} ($3d^9$) state toward a hole-doped, strongly correlated superconducting regime [11]. Similarly, the electron-doped side had been mapped out for cuprates by, e.g., substituting Nd^{3+} with Ce^{4+} in Nd_2CuO_4 [12,13]; cf. Refs. [14–16].

For nickelate superconductors, such as infinite-layer (IL) nickelates RNiO_2 [5,6] and Ruddlesden-Popper (RP) nickelates $\text{R}_{n+1}\text{Ni}_n\text{O}_{3n+1}$ [7–9,17,18], hole doping through

substituting the rare-earth cation R^{3+} by Sr^{2+} or Ca^{2+} is possible [6,17–21] and laid bare the enormous potential of nickelates. While hole doping of nickelates is straightforward, the lack of a robust route to electron doping has hindered a complete mapping of their phase diagram. This difficulty arises because substitutional doping requires higher-valence cations, i.e., tetravalent A-site ions. For LaNiO_3 [22] with Ni^{3+} just as in cuprates [13], this is possible by substituting La with Ce^{4+} . However, because the fourth electron ionic energy of Ce^{3+} is higher than the second ionization energy of Ni^{1+} for RP nickelates, this route is not possible.

Here, we propose a conceptually simple but feasible solution (see Fig. 1): achieve electron doping via wide-band-gap insulator intercalation in RP lanthanum oxides. The basic principle exploits the atomic and elementary versatility of RP phases, which consist of perovskite blocks separated by rocksalt layers. By inserting wide-gap insulating LaXO_3 blocks ($X = \text{Al, Ga, Sc}$) [23,24], which naturally form La_2XO_4 units in RP phase structures, the lattice introduces excess $(\text{LaO})^+$ layers. These act as effective electron donors, releasing electrons into adjacent transition-metal oxide planes. Unlike conventional chemical doping, this strategy does not introduce chemical

*Contact author: siliang@nwu.edu.cn

Published by the American Physical Society under the terms of the Creative Commons Attribution 4.0 International license. Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.

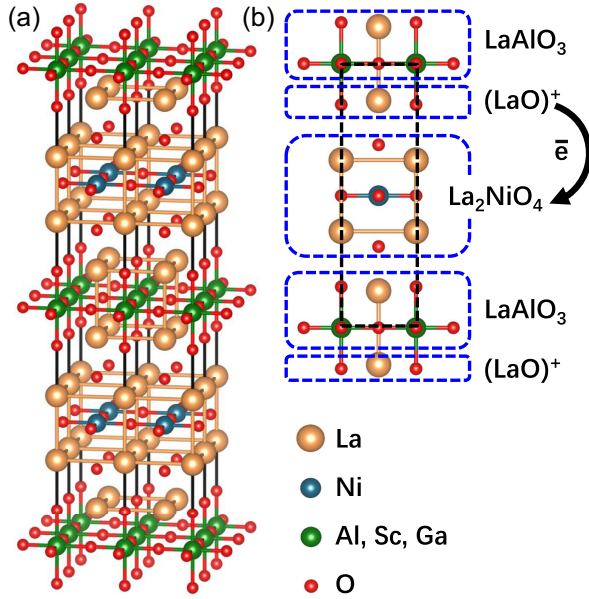


FIG. 1. (a) Structural schematic of $\text{La}_2\text{NiO}_4:\text{La}_2\text{XO}_4$ ($X = \text{Al}, \text{Sc}, \text{ or } \text{Ga}$); (b) Mechanism of intrinsic electron doping in La_2NiO_4 realized by inserting additional $(\text{LaO})^+$ layers. The black dashed line in (b) denotes the unit cell used for the DFT and DMFT calculations shown in Figs. 2(b)–2(d).

disorder at A and B sites; hence, it provides a defect- and disorder-free symmetry-preserving route to electron doping. This is very advantageous for stabilizing *fragile* emergent correlated states. We investigate this concept through first-principles and many-body calculations for $\text{La}_2\text{NiO}_4:\text{La}_2\text{XO}_4$ heterostructures.

Our density-functional theory (DFT) [25,26] and dynamical mean-field theory (DMFT) [27,28] calculations confirm significant charge transfer from the $\text{La}(\text{Al}, \text{Ga}, \text{Sc})\text{O}_3$ -derived blocks into NiO_2 layers, driving Ni toward $3d^9$ configurations in La_2NiO_4 units and electron doping $\text{La}_3\text{Ni}_2\text{O}_7$. Furthermore, many-body calculations identify $d_{x^2-y^2}$ -wave superconductivity (above 50 K) in $\text{La}_2\text{NiO}_4:\text{La}_2\text{AlO}_4$ even at ambient pressure. These results establish wide-band-gap intercalation as a promising strategy to access electron-doped nickelate. The proposed strategy may be extended to lanthanum manganites, cobaltates, or ruthenates, where the research on electron-doping effects still faces challenges, and even cuprates.

Method—The calculations in this Letter were primarily performed using DFT [25,26,29–34] for structural optimization and band structure analysis. The constrained random phase approximation [35–37] is employed for determining interaction parameters and DMFT [27,28,38–49] to account for local correlation effects. Additionally, the dynamical vertex approximation (D Γ A) [50–54], fluctuation exchange (FLEX) method [55–62], and dynamical cluster approximation (DCA) [63–67] were employed to study correlations beyond DMFT and to estimate the critical superconducting temperatures T_c . (Self-consistent) phonon calculations

(SCPH) [68–70] and first-principles molecular dynamics (AIMD) [71] simulations using on-the-fly machine-learned force fields [72,73] were carried out to assess the structural stability. Additional results, computational details, and parameter settings are provided in Supplemental Material Secs. I–IX [74].

Structure—We focus on RP-phase oxides $A_{x+1}B_x\text{O}_{3x+1}$ with $x = 1$, i.e., $A_2\text{BO}_4$. Many perovskite transition-metal oxides have been synthesized in this RP phase; prominent examples include Sr_2RuO_4 [75], La_2CuO_4 , and Sr_2TiO_4 [76]. These compounds feature $A_2\text{BO}_4$ layers stacked on top of each other. Often, they are synthesized by molecular beam epitaxy or pulsed laser deposition. For $x = \infty$, on the other hand, combinations of trivalent rare-earth cations (e.g., La^{3+}) with trivalent elements from the III A or III B group form wide-band-gap perovskite insulators such as LaAlO_3 (3.6 eV), LaGaO_3 (2.9 eV), and LaScO_3 (2.9 eV). For ABO_3 compounds, heterostructures or interfaces can be engineered when two materials share similar crystal structures and lattice constants. Consequently, when growing the $A_2\text{BO}_4$ —whose unit blocks contain an ABO_3 monolayer—it becomes possible to insert additional ABO_3 layers of varying type or thickness. Examples include $\text{Sr}_2\text{TiO}_4/\text{SrTiO}_3$ ($x = 1 + \infty$) interfaces [77] and the recently reported $\text{La}_2\text{NiO}_4/\text{La}_3\text{Ni}_2\text{O}_7$ heterostructure ($x = 1 + 2$) [78,79].

Following this reasoning, replacing every other unit block of La_2NiO_4 by La_2XO_4 yields structural analogs where La_2XO_4 ($\text{La}_3\text{X}_2\text{O}_7$) can be viewed as one (or two) unit cells of LaXO_3 plus an extra $(\text{LaO})^+$ layer. Here, La and O ions are expected to retain their $3+$ and $2-$ valence states, respectively. This introduces an extra electron into the La_2NiO_4 layer, provided that La and X ($\text{Al}, \text{Ga}, \text{ and } \text{Sc}$) are more ionic than Ni , as illustrated in Fig. 1(b). In Supplemental Material Secs. IX and X [74], we employed DFT, SCPH, and AIMD methods to perform phonon spectra, finite-temperature MD simulations, variable-composition structural searches, and constructed convex hulls. The results demonstrate that the $\text{La}_2\text{NiO}_4:\text{La}_2\text{AlO}_4$ heterostructure remains dynamically, chemically, and thermodynamically stable at even 300 K.

DFT bands—Let us start with the DFT band structure [Figs. 2(a) and 2(b)] and orbital occupations (Table I) of La_2NiO_4 with and without the intercalation of La_2XO_4 . For (undoped) La_2NiO_4 , Ni ions adopt a valence state of $2 + (3d^8)$, with fully occupied $\text{Ni-}t_{2g}$ and half-filled $\text{Ni-}e_g$ orbitals; see Table I. Because of the elongated octahedral field in the z direction and, thus, more distant (negatively charged) $\text{O-}2p_z$ orbitals, the $\text{Ni } d_{z^2}$ orbital is lower in energy than the $d_{x^2-y^2}$ orbital; see Fig. 2(a). Consistent with this, Table I shows an occupancy of 1.46 electron in d_{z^2} and 0.56 electron in $d_{x^2-y^2}$ in DFT. When La_2AlO_4 is intercalated [Fig. 2(b) and Table I], the additional $(\text{LaO})^+$ layers release roughly one electron to $\text{Ni-}3d_{z^2}$, leading to the occupation of $n \sim 1.91$ (1.93) in DFT (DMFT), while the

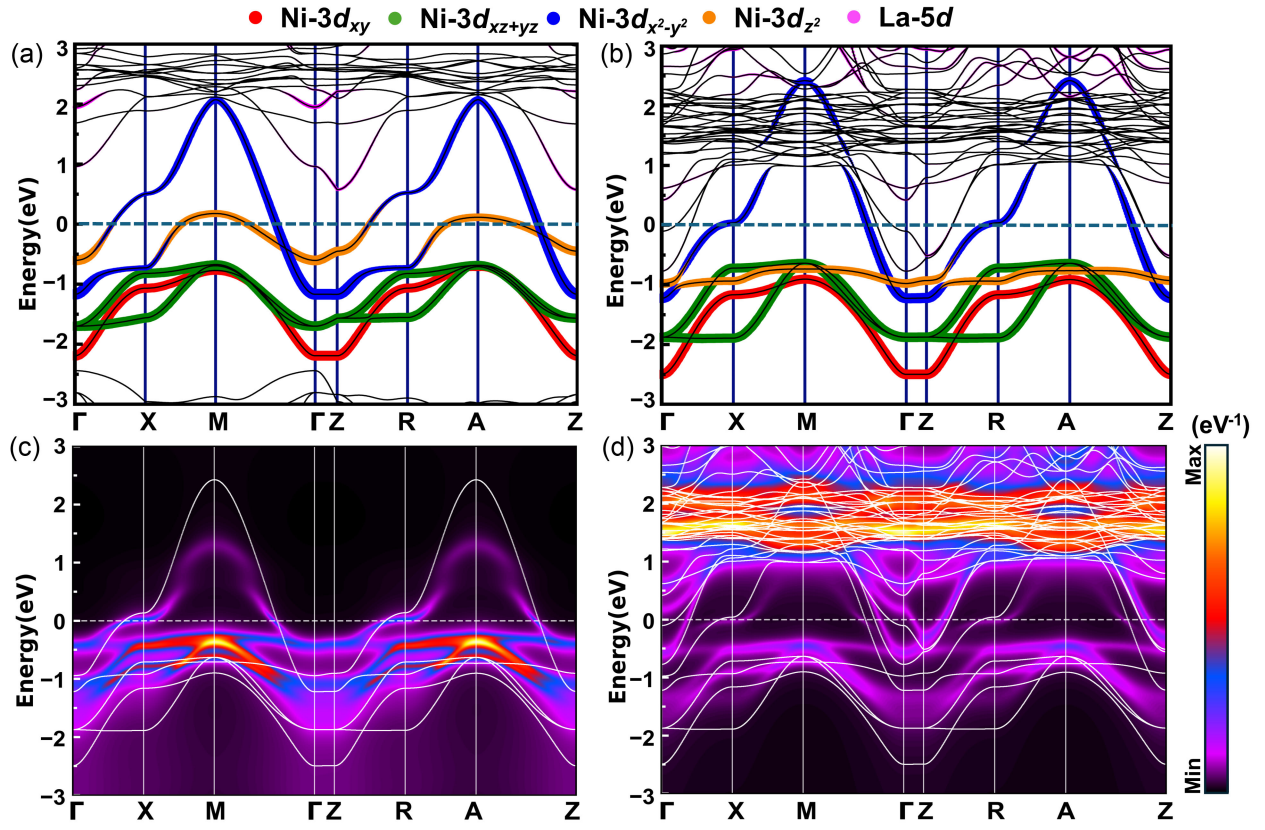


FIG. 2. Paramagnetic DFT band structure and orbital characters of (a) La_2NiO_4 and (b) $\text{La}_2\text{NiO}_4:\text{La}_2\text{AlO}_4$. Multiband DMFT k -resolved spectral functions $A(k, \omega)$ of $\text{La}_2\text{NiO}_4:\text{La}_2\text{AlO}_4$ with (c) Ni-3d-only model and (d) La-4f-5d+Ni-3d model.

$d_{x^2-y^2}$ occupation increases slightly to 0.65 (0.87) in DFT (DMFT). This corresponds to approximately one electron doping per Ni as in the sketch Fig. 1(b).

Similar electron-doping effects are observed for $\text{La}_2\text{NiO}_4:\text{La}_2\text{GaO}_4$ and $\text{La}_2\text{NiO}_4:\text{La}_2\text{ScO}_4$; the corresponding Table SI and Fig. S4 can be found in Supplemental Material [74] Secs. XI and XII. However, as the ionic size increases from Al via Ga to Sc, the in-plane lattice expands (see Table I), inducing a compressive strain in the z direction. This lowers the energy of the $d_{x^2-y^2}$

orbital, decreases its occupation, and increases the occupation of the d_{z^2} orbital. Importantly, in $\text{La}_2\text{NiO}_4:\text{La}_2\text{AlO}_4$, the Fermi surface exhibits quasisingle $d_{x^2-y^2}$ band character, with nearly full d_{z^2} occupancy and half-filled $d_{x^2-y^2}$, closely resembling cuprates such as La_2CuO_4 [80,81] and CaCuO_2 [82] and hydrogenated La_2NiO_4 [83]. At the $\Gamma = (0, 0, 0)$ and $Z = (0, 0, \pi)$ momenta, pocket bands of predominately La-5d character emerge but do not overlap with Ni- e_g bands. These pockets lead to the La occupation of

TABLE I. Occupation of Ni-3d and La-5d orbitals, out-of-plane Ni-O bond, and in-plane lattice constants (in unit of Å).

Materials Wannier projection basis	Method	Orbital occupancy					Structural parameters (Å)	
		d_{xy}	d_{xz}/d_{yz}	$d_{x^2-y^2}$	d_{z^2}	Average-La-5d	Out-of-plane Ni-O	In-plane lattice constant
La_2NiO_4	DFT	1.98	2.00	0.56	1.46	...	2.37	3.80
(Ni-3d only)	DMFT	2.00	2.00	1.00	1.00	...		
$\text{La}_2\text{NiO}_4:\text{La}_2\text{AlO}_4$	DFT	1.95	1.92	0.65	1.91	0.16	2.56	3.76
(La-5d + Ni-3d)	DMFT	1.95	1.93	0.87	1.93	0.10		
$\text{La}_2\text{NiO}_4:\text{La}_2\text{GaO}_4$	DFT	1.97	1.96	0.67	1.90	0.13	2.50	3.80
(La-5d + Ni-3d)	DMFT	1.98	1.96	0.90	1.93	0.06		
$\text{La}_2\text{NiO}_4:\text{La}_2\text{ScO}_4$	DFT	1.94	1.92	0.76	1.81	0.16	2.44	3.94
(La-5d + Ni-3d)	DMFT	1.96	1.94	1.01	1.71	0.11		

0.16 (0.10) electrons/La in DFT (DMFT) and self-dope the $\text{Ni-}3d_{x^2-y^2}$ band, analogous to IL nickelates [84,85]. Moreover, spin-polarized DFT + U calculations reveal that the proposed compounds exhibit (in-plane) G -type antiferromagnetism, analogous to that observed in 2D cuprates (see Supplemental Material Sec. XI [74]).

In addition to the DFT bands, the charge transfer effect induced by the heterostructure is further confirmed by DFT density of states (DOS), Mulliken population, and Bader charge analysis (see Supplemental Material Sec. XIII [74]).

The mechanism of electron doping can be extended to other RP phase oxides, such as the recently discovered superconductor $\text{La}_3\text{Ni}_2\text{O}_7$ [7–9,17,18]. For $\text{La}_3\text{Ni}_2\text{O}_7$, we constructed an $\text{La}_3\text{Ni}_2\text{O}_7:\text{La}_3\text{Al}_2\text{O}_7$ superlattice. Figures 3(a) and 3(b) show the DFT bands with a pronounced downward shift of the $\text{Ni-}e_g$ orbitals, corresponding to an electron doping of the low-energy Ni orbitals. This demonstrates the versatility of our electron-doping approach and its applicability to diverse RP nickelates and other oxides.

Unlike conventional approaches that rely on the potential difference between B and B' cations at $\text{ABO}_3/\text{AB}'\text{O}_3$ heterostructure to induce charge transfer and self-doping [86–88], the gateway we propose avoids introducing additional bonding associated with electron or hole doping, which typically alters the electronic and magnetic structures.

Correlations—Next, we turn to the effect of correlations, starting with the strong local correlations that can be captured by DMFT; the corresponding computational details are provided in Supplemental Material Sec. III [74]. As theoretically [89] and experimentally [90,91] established for both infinite- and finite-layer nickelates as well as for cuprates, quasi-2D superconductivity is primarily governed by the nearly half-filled Fermi surface derived from $\text{Ni-}3d_{x^2-y^2}$ single-band. The slightly occupied pocket(s) at Γ and A points are considered to play, as in nickelates, a minor role of an electron reservoir (hole donor) and not to be decisive for superconductivity.

We perform DFT + DMFT calculations for two different low-energy models: including all $\text{Ni-}3d$ orbitals (only)

[Fig. 2(c)] and a $\text{La-}4f + \text{La-}5d + \text{Ni-}3d$ model which also includes the $\text{La-}4f$ and $5d$ orbitals [Fig. 2(d)] [94]. In the $\text{Ni-}3d$ (only) case, both t_{2g} and d_{z^2} bands shift upward by ~ 1 eV, while the Fermi surface remains dominated by the $d_{x^2-y^2}$ orbital. The $\text{La-}4f\text{-}5d + \text{Ni-}3d$ model exhibits similar characteristics; although the Γ and Z pockets shift upward, they still cross the Fermi energy [see Fig. 4(b) for DFT and DMFT Fermi surface and the enhanced occupation in $\text{Ni-}3d_{x^2-y^2}$], suggesting that correlations suppress the self-doping effect between $\text{Ni-}3d$ and $\text{La-}5d$ [these pockets are not part of the $\text{Ni-}3d$ (only) model]. The calculated $d_{x^2-y^2}$ effective electron masses $m^*/m = (1/Z) = 1 - [\partial \text{Im} \Sigma(i\omega_n)/\partial i\omega_n]|_{i\omega_n \rightarrow 0}$ are with 2.8 ($\text{Ni-}3d$) and 3.1 ($\text{La-}4f\text{-}5d + \text{Ni-}3d$) quite similar for the two models, confirming that the $\text{Ni-}3d$ orbital retains its distinct electronic character in both models and is largely decoupled from other orbital contributions.

Superconductivity in $\text{La}_2\text{NiO}_4:\text{La}_2\text{AlO}_4$ —Going even beyond the DMFT correlations, we compute the superconducting critical temperature (T_c) of $\text{La}_2\text{NiO}_4:\text{La}_2\text{AlO}_4$ using three different methods: D Γ A, FLEX, and DCA. For these more involved calculations, we use a single-band tight-binding Hamiltonian obtained from a Wannier projection onto the only correlated band crossing the Fermi energy: the $\text{Ni-}3d_{x^2-y^2}$ band. Computational details are provided in Supplemental Material Secs. IV–VIII [74]. As summarized in Table I, the DFT + DMFT calculations ($\text{La-}4f + \text{La-}5d + \text{Ni-}3d$ model) yield an electron occupancy of $n = 0.87$ for the $\text{Ni-}3d_{x^2-y^2}$ orbital. This filling was used in the D Γ A, FLEX, and DCA calculations to mimic the effect of the pockets and is consistent with the optimal carrier concentration (~ 0.85) predicted in a previous study [89]. For FLEX and D Γ A, we also examined additional fillings ($n = 0.80$ and 0.90 for FLEX and $n = 0.80$ and 0.95 for D Γ A). Figure 4(a) shows the temperature dependence of the superconducting eigenvalues λ_{SC} as a function of T for different n . D Γ A yields T_c ($\lambda_{\text{SC}} = 1$) values of 53 and 62 K for $n = 0.87$ and $n = 0.95$, respectively, higher than current IL nickelates [89,92,93]. This high T_c can be traced back to the reduced

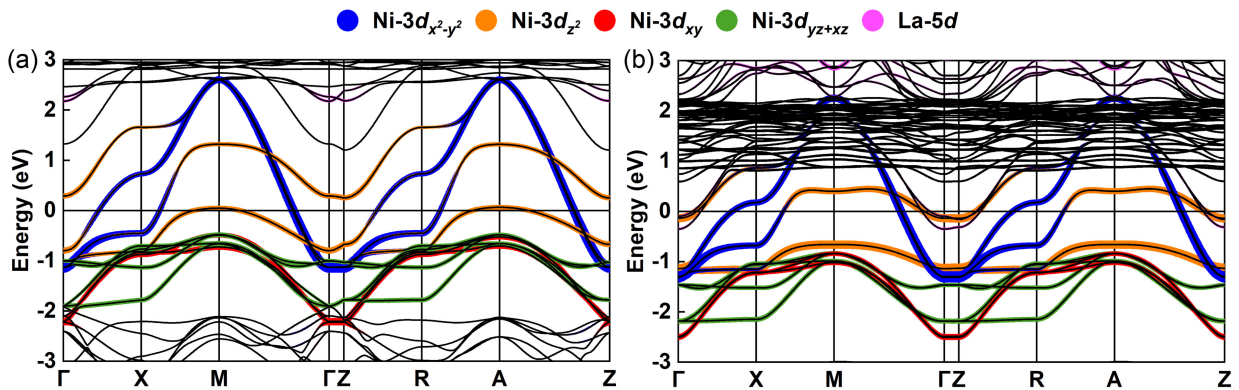


FIG. 3. Paramagnetic DFT band structure and orbital characters of (a) $\text{La}_3\text{Ni}_2\text{O}_7$ and (b) $\text{La}_3\text{Ni}_2\text{O}_7:\text{La}_3\text{Al}_2\text{O}_7$.

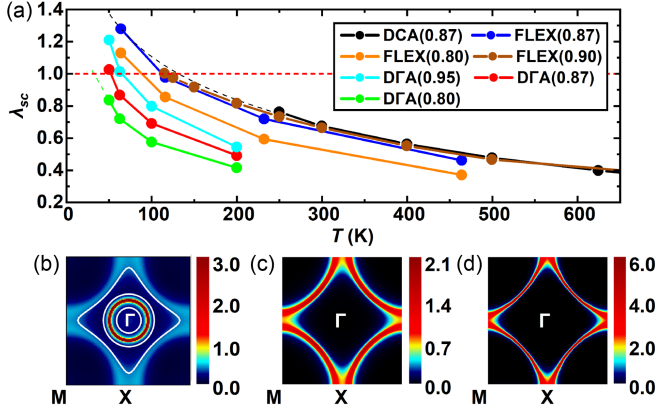


FIG. 4. (a) Leading d -wave superconducting λ_{SC} eigenvalue as a function of temperature using fitting form of $\lambda_{SC} \approx a - b \ln(T)$ as in previous publications [83,89,95]; Fermi surface at $k_z = 0$ computed by (b) DFT (white lines) and DMFT (colorful spectra), (c) FLEX, and (d) DGA. The FLEX and DGA Fermi surface are computed by the momentum dependence of the imaginary part of the Green function $[-\text{Im} G(k, \omega_0)/\pi]$ at lowest Matsubara frequency $\omega_0 = \pi k_B T$, $T = 53$ K and $n = 0.87$. Note that the DFT Fermi surfaces in (b) displays additional Γ pockets that are taken into account in DGA and FLEX only through a reduced filling.

in-plane lattice constant ($3.76 \text{ \AA}$) which weakens correlations ($U \approx 5t - 6t$ instead of $7t - 8t$ for LaNiO_2 [85,95,96]) and makes $\text{La}_2\text{NiO}_4:\text{La}_2\text{AlO}_4$ analogous to $4d$ palladates [95].

The same tendency is observed in FLEX with even a T_c of 103 and 115 K at $n = 0.87$ and $n = 0.90$, respectively; and DCA with cutting-edge $N_c = 12$ cluster sites predicts a similar T_c of 127 K. Taking all three many-body approaches together and even with the most conservative DGA T_c , we can conclude with quite some confidence that $\text{La}_2\text{NiO}_4:\text{La}_2\text{AlO}_4$ is a d -wave superconductor with a high T_c , which we predict to exceed that of IL nickelates. It should be noted that, during the synthesis of the proposed heterostructures, inversion symmetry (centrosymmetry) breaking may introduce additional bands near the Fermi level into the minimal low-energy model, potentially leading to multiband superconducting pairing [97]. In addition, we discussed the effects of lattice, structure, and strain on the electronic structure of the heterostructures [98] in Supplemental Material Sec. XIV [74].

Finally, the Fermi surfaces obtained from the many-body DMFT, FLEX, and DGA methods exhibit remarkable similarity to previous results for states where superconductivity and a well-defined holelike Fermi surface emerges [95]. Specifically, Figs. 4(c) and 4(d) show a characteristic shape with pronounced strong momentum-dependent damping at the many-body level instead of the noninteracting DFT Fermi surface in Fig. 4(b). Noteworthy, electronic correlations induce a Lifshitz transition from an electron Fermi surface in DFT to a

holelike Fermi surface. Our model parameters ($t'/t = -0.20$ and $t''/t = 0.10$) of $\text{La}_2\text{NiO}_4:\text{La}_2\text{AlO}_4$ indeed fall within the optimal regime identified in the previous study ($t'/t = -0.22$ and $t''/t = 0.14$) [95], suggesting that this system possesses strong potential for high- T_c superconductivity.

Conclusions—Lanthanum nickelates have recently reemerged at the focus of condensed matter research, following the discovery of unconventional cupratelike superconductivity. However, electron doping in nickelates remains much more difficult than in cuprates due to the highly ionic nature of Ni and limited availability of suitable elements. In contrast, in cuprates, the low ionization energy of their A-site elements allows Ce to adopt a $4+$ valence state, enabling electron doping.

In this Letter, we proposed intercalation of the insulating RP nickelates as a promising route to achieve electron doping. Electron doping was confirmed using DFT and DMFT calculations: In $\text{La}_2\text{NiO}_4:\text{La}_2\text{AlO}_4$, a $3d^{9-\delta}$ ($\delta \sim 0.13$) valence state was realized, demonstrating that the Ni e_g orbital in La_2NiO_4 is effectively doped with electron(s) from the additional $(\text{LaO})^+$ layer(s). We also demonstrated the feasibility of this approach for $\text{La}_3\text{Ni}_2\text{O}_7$. Let us emphasize that the approach is not at all restricted to nickelates. It is widely applicable to introducing electron doping in other RP-phase oxides and very promising for, e.g., cuprates such as La_2CuO_4 and ruthenates such as Sr_2RuO_4 .

Subsequent many-body calculations, based on a simplified $\text{Ni-}3d_{x^2-y^2}$ model including correlation effects for the doped La_2NiO_4 layers, reveal that the electron-doped compounds host high- T_c $d_{x^2-y^2}$ -wave superconductivity, as shown by DGA, DCA, and FLEX. Compared to IL nickelate superconductors, $\text{La}_2\text{NiO}_4:\text{La}_2\text{AlO}_4$ exhibits a higher T_c due to the smaller in-plane lattice constant [that is close to $3.868 \text{ \AA}$ of LSAT: $(\text{LaAlO}_3)_{0.3}(\text{Sr}_2\text{TaAlO}_6)_{0.7}$]. This, in turn, reduces correlations and (antiferromagnetic) spin fluctuations and, thus, enhances T_c . Furthermore, due to the large La pockets, $\text{La}_2\text{NiO}_4:\text{La}_2\text{AlO}_4$ naturally resides in the optimal doping regime of superconductivity in the two-dimensional Hubbard model even without any additional doping.

In parallel to the charge-transfer mechanism proposed here, recent work [98] has demonstrated that geometrical effects—such as varying the thickness ratio of quantum wells in superlattices—can serve as an effective tuning parameter for controlling multiband superconductivity and achieving a multigap superconducting state. These findings suggest that a combination of charge transfer (chemical doping) and geometrical engineering could provide even greater flexibility in designing and optimizing the superconducting state in RP-phase nickelate heterostructures.

Acknowledgments—L. S. acknowledges support from the National Natural Science Foundation of China

(Grant No. 12422407) and the Key Research and Development Program of Shaanxi (2024QY2-GJHX-42). K. H. and L. S. acknowledge funding through the Austrian Science Funds (FWF) Project [Grant No. DOI 10.55776/I5398] and the European Research Council through ERC-2024-ADG RealSuper Project DOI 10.3030/101201037. W. W. acknowledges the funding from the China Scholarship Council (CSC). G. J. and M. J. acknowledge the support of the National Natural Science Foundation of China (Grant No. 12174278). N. W. acknowledges support through the Deutsche Forschungsgemeinschaft (DFG) funded SFB 1170 (“Tocotronics,” Project No. 258499086). N. W. and K. H. acknowledge support from the DFG research unit FOR5249 (“QUAST,” Project No. 449872909) and the FWF-funded QUAST (Sub) project [DOI 10.55776/KIN2563725]. M. K. acknowledges support from JSPS KAKENHI Grants No. JP23H03817, No. JP24K17014, and No. JP25K00961. Calculations have been done on the National Supercomputing Center in Northwest University (Xi’an), the Vienna Scientific Cluster (VSC), Soochow University, and the Research Institute for Information Technology, Kyushu University (General Projects). This project is funded in part by the European Union. Views and opinions expressed are, however, those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council Executive Agency

Data availability—The data that support the findings of this article are openly available [99].

- [1] J. G. Bednorz and K. A. Müller, Possible high- T_c superconductivity in the Ba – La – Cu – O system, *Z. Phys. B* **64**, 189 (1986).
- [2] P. W. Anderson, *The Theory of Superconductivity in the High- T_c Cuprate Superconductors* (Princeton University Press, Princeton, NJ, 1997).
- [3] C. C. Tsuei and J. R. Kirtley, Pairing symmetry in cuprate superconductors, *Rev. Mod. Phys.* **72**, 969 (2000).
- [4] A. Damascelli, Z. Hussain, and Z.-X. Shen, Angle-resolved photoemission studies of the cuprate superconductors, *Rev. Mod. Phys.* **75**, 473 (2003).
- [5] D. Li, K. Lee, B. Y. Wang, M. Osada, S. Crossley, H. R. Lee, Y. Cui, Y. Hikita, and H. Y. Hwang, Superconductivity in an infinite-layer nickelate, *Nature (London)* **572**, 624 (2019).
- [6] S. W. Zeng, C. J. Li, L. E. Chow, Y. Cao, Z. T. Zhang, C. S. Tang, X. M. Yin, Z. S. Lim, J. X. Hu, P. Yang *et al.*, Superconductivity in infinite-layer nickelate $\text{La}_{1-x}\text{Ca}_x\text{NiO}_2$ thin films, *Sci. Adv.* **8**, eabl9927 (2022).
- [7] H. Sun, M. Huo, X. Hu, J. Li, Z. Liu, Y. Han, L. Tang, Z. Mao, P. Yang, B. Wang *et al.*, Signatures of superconductivity near 80 K in a nickelate under high pressure, *Nature (London)* **621**, 493 (2023).
- [8] D. Zhao, Y. Zhou, M. Huo, Y. Wang, L. Nie, Y. Yang, J. Ying, M. Wang, T. Wu, and X. Chen, Pressure-enhanced spin-density-wave transition in double-layer nickelate $\text{La}_3\text{Ni}_2\text{O}_{7-\delta}$, *Sci. Bull.* **70**, 1239 (2025).
- [9] G. Wang, N. N. Wang, X. L. Shen, J. Hou, L. Ma, L. F. Shi, Z. A. Ren, Y. D. Gu, H. M. Ma, P. T. Yang, Z. Y. Liu, H. Z. Guo, J. P. Sun, G. M. Zhang, S. Calder, J.-Q. Yan, B. S. Wang, Y. Uwatoko, and J.-G. Cheng, Pressure-induced superconductivity in polycrystalline $\text{La}_3\text{Ni}_2\text{O}_{7-\delta}$, *Phys. Rev. X* **14**, 011040 (2024).
- [10] P. W. Anderson, The resonating valence bond state in La_2CuO_4 and superconductivity, *Science* **235**, 1196 (1987).
- [11] F. C. Zhang and T. M. Rice, Effective hamiltonian for the superconducting Cu oxides, *Phys. Rev. B* **37**, 3759 (1988).
- [12] H. Takagi, S. Uchida, and Y. Tokura, Superconductivity produced by electron doping in CuO_2 -layered compounds, *Phys. Rev. Lett.* **62**, 1197 (1989).
- [13] N. P. Armitage, P. Fournier, and R. L. Greene, Progress and perspectives on electron-doped cuprates, *Rev. Mod. Phys.* **82**, 2421 (2010).
- [14] R. J. Birgeneau, C. Stock, J. M. Tranquada, and K. Yamada, Magnetic neutron scattering in hole-doped cuprate superconductors, *J. Phys. Soc. Jpn.* **75**, 111003 (2006).
- [15] W. S. Lee, J. J. Lee, E. A. Nowadnick, S. Gerber, W. Tabis, S. W. Huang, V. N. Strocov, E. M. Motoyama, G. Yu, B. Moritz *et al.*, Asymmetry of collective excitations in electron-and hole-doped cuprate superconductors, *Nat. Phys.* **10**, 883 (2014).
- [16] P. Abbamonte, L. Venema, A. Rusydi, G. A. Sawatzky, G. Logvenov, and I. Bozovic, A structural probe of the doped holes in cuprate superconductors, *Science* **297**, 581 (2002).
- [17] E. K. Ko, Y. J. Yu, Y. D. Liu, L. Bhatt, J. R. Li, V. Thampy, C.-T. Kuo, B. Y. Wang, Y. H. Lee, K. H. Lee *et al.*, Signatures of ambient pressure superconductivity in thin film $\text{La}_3\text{Ni}_2\text{O}_7$, *Nature (London)* **638**, 935 (2025).
- [18] G. D. Zhou, W. Lv, H. Wang, Z. H. Nie, Y. Q. Chen, Y. Y. Li, H. L. Huang, W.-Q. Chen, Y.-J. Sun, Q.-K. Xue *et al.*, Ambient-pressure superconductivity onset above 40 K in $(\text{La}, \text{Pr})_3\text{Ni}_2\text{O}_7$ films, *Nature (London)* **640**, 641 (2025).
- [19] D. F. Li, B. Y. Wang, K. H. Lee, S. P. Harvey, M. Osada, B. H. Goodge, L. F. Kourkoutis, and H. Y. Hwang, Superconducting dome in $\text{Nd}_{1-x}\text{Sr}_x\text{NiO}_2$ infinite layer films, *Phys. Rev. Lett.* **125**, 027001 (2020).
- [20] M. Osada, B. Y. Wang, B. H. Goodge, S. P. Harvey, K. H. Lee, D. F. Li, L. F. Kourkoutis, and H. Y. Hwang, Nickelate superconductivity without rare-earth magnetism: $(\text{La}, \text{Sr})\text{NiO}_2$, *Adv. Mater.* **33**, 2104083 (2021).
- [21] Y. X. Wang, K. Jiang, J. J. Ying, T. Wu, J. G. Cheng, J. P. Hu, and X. H. Chen, Recent progress in nickelate superconductors, *Natl. Sci. Rev.* **12**, nwaf373 (2025).
- [22] P. Puphal, V. Sundaramurthy, V. Zimmermann, K. Küster, U. Starke, M. Isobe, B. Keimer, and M. Hepting, Phase formation in hole-and electron-doped rare-earth nickelate single crystals, *APL Mater.* **11**, 081107 (2023).
- [23] M. Rizwan, S. Gul, T. Iqbal, U. Mushtaq, M. H. Farooq, M. Farman, R. Bibi, and M. Ijaz, A review on perovskite lanthanum aluminate (LaAlO_3), its properties and applications, *Mater. Res. Express* **6**, 112001 (2019).

- [24] D. Lybye, F. W. Poulsen, and M. Mogensen, Conductivity of A-site and B-site doped LaAlO_3 , LaGaO_3 , LaScO_3 and LaInO_3 perovskites, *Solid State Ionics* **128**, 91 (2000).
- [25] P. Hohenberg and W. Kohn, Inhomogeneous electron gas, *Phys. Rev.* **136**, B864 (1964).
- [26] W. Kohn and L. J. Sham, Self-consistent equations including exchange and correlation effects, *Phys. Rev.* **140**, A1133 (1965).
- [27] W. Metzner and D. Vollhardt, Correlated lattice fermions in $d = \infty$ dimensions, *Phys. Rev. Lett.* **62**, 324 (1989).
- [28] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions, *Rev. Mod. Phys.* **68**, 13 (1996).
- [29] P. E. Blöchl, Projector augmented-wave method, *Phys. Rev. B* **50**, 17953 (1994).
- [30] G. Kresse and J. Furthmüller, Efficiency of *ab-initio* total energy calculations for metals and semiconductors using a plane-wave basis set, *Comput. Mater. Sci.* **6**, 15 (1996).
- [31] G. Kresse and J. Furthmüller, Efficient iterative schemes for *ab initio* total-energy calculations using a plane-wave basis set, *Phys. Rev. B* **54**, 11169 (1996).
- [32] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, and J. Luitz, WIEN2k, An augmented plane wave + local orbitals program for calculating crystal properties, (2001).
- [33] K. Schwarz, P. Blaha, and G. K. H. Madsen, Electronic structure calculations of solids using the WIEN2k package for material sciences, *Comput. Phys. Commun.* **147**, 71 (2002).
- [34] J. P. Perdew, K. Burke, and M. Ernzerhof, Generalized gradient approximation made simple, *Phys. Rev. Lett.* **77**, 3865 (1996).
- [35] T. Miyake and F. Aryasetiawan, Screened coulomb interaction in the maximally localized Wannier basis, *Phys. Rev. B* **77**, 085122 (2008).
- [36] L. Si, P. T. Liu, and C. Franchini, Evolution of the coulomb interactions in correlated transition-metal perovskite oxides from the constrained random phase approximation, *Phys. Rev. Mater.* **9**, 015001 (2025).
- [37] L. Si, W. Xiao, J. Kaufmann, J. M. Tomczak, Y. Lu, Z. C. Zhong, and K. Held, Topotactic hydrogen in nickelate superconductors and akin infinite-layer oxides ABO_2 , *Phys. Rev. Lett.* **124**, 166402 (2020).
- [38] G. H. Wannier, The structure of electronic excitation levels in insulating crystals, *Phys. Rev.* **52**, 191 (1937).
- [39] N. Marzari, A. A. Mostofi, J. R. Yates, I. Souza, and D. Vanderbilt, Maximally localized Wannier functions: Theory and applications, *Rev. Mod. Phys.* **84**, 1419 (2012).
- [40] A. A. Mostofi, J. R. Yates, Y.-S. Lee, I. Souza, D. Vanderbilt, and N. Marzari, Wannier90: A tool for obtaining maximally-localised Wannier functions, *Comput. Phys. Commun.* **178**, 685 (2008).
- [41] J. Kuneš, R. Arita, P. Wissgott, A. Toschi, H. Ikeda, and K. Held, Wien2wannier: From linearized augmented plane waves to maximally localized Wannier functions, *Comput. Phys. Commun.* **181**, 1888 (2010).
- [42] A. I. Liechtenstein, V. I. Anisimov, and J. Zaanen, Density-functional theory and strong interactions: Orbital ordering in Mott-Hubbard insulators, *Phys. Rev. B* **52**, R5467 (1995).
- [43] V. I. Anisimov, I. V. Solovyev, M. A. Korotin, M. T. Czyżyk, and G. A. Sawatzky, Density-functional theory and NiO photoemission spectra, *Phys. Rev. B* **48**, 16929 (1993).
- [44] E. Gull, A. J. Millis, A. I. Lichtenstein, A. N. Rubtsov, M. Troyer, and P. Werner, Continuous-time Monte Carlo methods for quantum impurity models, *Rev. Mod. Phys.* **83**, 349 (2011).
- [45] N. Parragh, A. Toschi, K. Held, and G. Sangiovanni, Conserved quantities of $SU(2)$ -invariant interactions for correlated fermions and the advantages for quantum Monte Carlo simulations, *Phys. Rev. B* **86**, 155158 (2012).
- [46] M. Wallerberger, A. Hausoel, P. Gunacker, A. Kowalski, N. Parragh, F. Goth, K. Held, and G. Sangiovanni, w2dynamics: Local one- and two-particle quantities from dynamical mean field theory, *Comput. Phys. Commun.* **235**, 388 (2019).
- [47] J. E. Gubernatis, M. Jarrell, R. N. Silver, and D. S. Sivia, Quantum Monte Carlo simulations and maximum entropy: Dynamics from imaginary-time data, *Phys. Rev. B* **44**, 6011 (1991).
- [48] A. W. Sandvik, Stochastic method for analytic continuation of quantum Monte Carlo data, *Phys. Rev. B* **57**, 10287 (1998).
- [49] J. Kaufmann and K. Held, ANA_CONT: Python package for analytic continuation, *Comput. Phys. Commun.* **282**, 108519 (2023).
- [50] A. Galler, P. Thunström, J. Kaufmann, M. Pickem, J. M. Tomczak, and K. Held, The *ab initio* DGA project v1. 0: Non-local correlations beyond and susceptibilities within dynamical mean-field theory, *Comput. Phys. Commun.* **245**, 106847 (2019).
- [51] K. Held, A. A. Katanin, and A. Toschi, Dynamical vertex approximation: An introduction, *Prog. Theor. Phys. Suppl.* **176**, 117 (2008).
- [52] G. Rohringer, H. Hafermann, A. Toschi, A. A. Katanin, A. E. Antipov, M. I. Katsnelson, A. I. Lichtenstein, A. N. Rubtsov, and K. Held, Diagrammatic routes to nonlocal correlations beyond dynamical mean field theory, *Rev. Mod. Phys.* **90**, 025003 (2018).
- [53] M. Kitatani, T. Schäfer, H. Aoki, and K. Held, Why the critical temperature of high- T_c cuprate superconductors is so low: The importance of the dynamical vertex structure, *Phys. Rev. B* **99**, 041115(R) (2019).
- [54] A. Toschi, A. A. Katanin, and K. Held, Dynamical vertex approximation: A step beyond dynamical mean-field theory, *Phys. Rev. B* **75**, 045118 (2007).
- [55] M. Kitatani, R. Arita, T. Schäfer, and K. Held, Strongly correlated superconductivity with long-range spatial fluctuations, *J. Phys. Mater.* **5**, 034005 (2022).
- [56] N. E. Bickers, D. J. Scalapino, and S. R. White, Conserving approximations for strongly correlated electron systems: Bethe-salpeter equation and dynamics for the Two-Dimensional Hubbard model, *Phys. Rev. Lett.* **62**, 961 (1989).
- [57] N. E. Bickers and S. R. White, Conserving approximations for strongly fluctuating electron systems. II. Numerical results and parquet extension, *Phys. Rev. B* **43**, 8044 (1991).
- [58] N. Witt, E. G. C. P. van Loon, T. Nomoto, R. Arita, and T. O. Wehling, Efficient fluctuation-exchange approach to low-temperature spin fluctuations and superconductivity: From

- the Hubbard model to $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$, *Phys. Rev. B* **103**, 205148 (2021).
- [59] N. Witt, L. Si, J. M. Tomczak, K. Held, and T. O. Wehling, No superconductivity in $\text{Pb}_9\text{Cu}_1(\text{PO}_4)_6\text{O}$ found in orbital and spin fluctuation exchange calculations, *SciPost Phys.* **15**, 197 (2023).
- [60] J. Li, M. Wallerberger, N. Chikano, C.-N. Yeh, E. Gull, and H. Shinaoka, Sparse sampling approach to efficient *ab initio* calculations at finite temperature, *Phys. Rev. B* **101**, 035144 (2020).
- [61] H. Shinaoka, J. Otsuki, M. Ohzeki, and K. Yoshimi, Compressing Green's function using intermediate representation between imaginary-time and real-frequency domains, *Phys. Rev. B* **96**, 035147 (2017).
- [62] M. Wallerberger, S. Badr, S. Hoshino, S. Huber, F. Kakizawa, T. Koretsune, Y. Nagai, K. Nogaki, T. Nomoto, H. Mori *et al.*, SPARSE-IR: Optimal compression and sparse sampling of many-body propagators, *SoftwareX* **21**, 101266 (2023).
- [63] M. H. Hettler, A. N. Tahvildar-Zadeh, M. Jarrell, T. Pruschke, and H. R. Krishnamurthy, Nonlocal dynamical correlations of strongly interacting electron systems, *Phys. Rev. B* **58**, R7475 (1998).
- [64] E. Gull, P. Werner, O. Parcollet, and M. Troyer, Continuous-time auxiliary-field Monte Carlo for quantum impurity models, *Europhys. Lett.* **82**, 57003 (2008).
- [65] T. A. Maier, M. S. Jarrell, and D. J. Scalapino, Structure of the pairing interaction in the two-dimensional Hubbard model, *Phys. Rev. Lett.* **96**, 047005 (2006).
- [66] T. A. Maier, M. Jarrell, and D. J. Scalapino, Pairing interaction in the two-dimensional Hubbard model studied with a dynamic cluster quantum Monte Carlo approximation, *Phys. Rev. B* **74**, 094513 (2006).
- [67] T. A. Maier, M. Jarrell, T. Pruschke, and M. H. Hettler, Quantum cluster theories, *Rev. Mod. Phys.* **77**, 1027 (2005).
- [68] A. Togo and I. Tanaka, First principles phonon calculations in materials science, *Scr. Mater.* **108**, 1 (2015).
- [69] T. Tadano, Y. Gohda, and S. Tsuneyuki, Impact of rattlers on thermal conductivity of a thermoelectric clathrate: A first-principles study, *Phys. Rev. Lett.* **114**, 095501 (2015).
- [70] T. Tadano and S. Tsuneyuki, Self-consistent phonon calculations of lattice dynamical properties in cubic SrTiO_3 with first-principles anharmonic force constants, *Phys. Rev. B* **92**, 054301 (2015).
- [71] G. Kresse and J. Hafner, *Ab initio* molecular dynamics for open-shell transition metals, *Phys. Rev. B* **48**, 13115 (1993).
- [72] R. Jinnouchi, J. Lahnsteiner, F. Karsai, G. Kresse, and M. Bokdam, Phase transitions of hybrid perovskites simulated by machine-learning force fields trained on the fly with bayesian inference, *Phys. Rev. Lett.* **122**, 225701 (2019).
- [73] R. Jinnouchi, F. Karsai, and G. Kresse, On-the-fly machine learning force field generation: Application to melting points, *Phys. Rev. B* **100**, 014105 (2019).
- [74] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/qp4p-x6g3> for additional results and computational details of DFT, DMFT, cRPA, DGA, FLEX, DCA, and AIMD calculations.
- [75] G. M. I. Luke, Y. Fudamoto, K. M. Kojima, M. I. Larkin, J. Merrin, B. Nachumi, Y. J. Uemura, Y. Maeno, Z. Q. Mao, Y. Mori *et al.*, Time-reversal symmetry-breaking superconductivity in Sr_2RuO_4 , *Nature (London)* **394**, 558 (1998).
- [76] K. T. Jacob and G. Rajitha, Thermodynamic properties of strontium titanates: Sr_2TiO_4 , $\text{Sr}_3\text{Ti}_2\text{O}_7$, $\text{Sr}_4\text{Ti}_3\text{O}_{10}$, and SrTiO_3 , *J. Chem. Thermodyn.* **43**, 51 (2011).
- [77] J. Li, X.-G. Tang, Q.-X. Liu, Y.-P. Jiang, W.-H. Li, and Z.-X. Tang, Interfacial resistive switching properties of $\text{Sr}_2\text{TiO}_4/\text{SrTiO}_3$ heterojunction thin films prepared via sol-gel process, *Ceram. Int.* **47**, 18808 (2021).
- [78] M. Z. Shi, D. Peng, K. B. Fan, Z. F. Xing, S. H. Yang, Y. Z. Wang, H. P. Li, R. Q. Wu, M. Du, B. H. Ge *et al.*, Pressure induced superconductivity in hybrid Ruddlesden-Popper $\text{La}_5\text{Ni}_3\text{O}_{11}$ single crystals, *Nat. Phys.* **21**, 1780 (2025).
- [79] F. Y. Li, N. Guo, Q. Zheng, Y. Shen, S. L. Wang, Q. H. Cui, C. Liu, S. P. Wang, X. T. Tao, G.-M. Zhang, and J. J. Zhang, Design and synthesis of three-dimensional hybrid Ruddlesden-Popper nickelate single crystals, *Phys. Rev. Mater.* **8**, 053401 (2024).
- [80] C. Lane, J. W. Furness, I. G. Buda, Y. B. Zhang, R. S. Markiewicz, B. Barbiellini, J. W. Sun, and A. Bansil, Antiferromagnetic ground state of La_2CuO_4 : A parameter-free *ab initio* description, *Phys. Rev. B* **98**, 125140 (2018).
- [81] M. T. Czyżyk and G. A. Sawatzky, Local-density functional and on-site correlations: The electronic structure of La_2CuO_4 and LaCuO_3 , *Phys. Rev. B* **49**, 14211 (1994).
- [82] J. Karp, A. S. Botana, M. R. Norman, H. Park, M. Zingl, and A. Millis, Many-body electronic structure of NdNiO_2 and CaCuO_2 , *Phys. Rev. X* **10**, 021061 (2020).
- [83] Y. Gao, W. F. Wu, Z. X. Liu, K. Held, and L. Si, Topotactical hydrogen induced single-band *d*-wave superconductivity in La_2NiO_4 , *Phys. Rev. Lett.* **135**, 026002 (2025).
- [84] H. Sakakibara, H. Usui, K. Suzuki, T. Kotani, H. Aoki, and K. Kuroki, Model construction and a possibility of cuprate-like pairing in a new d^9 nickelate superconductor $(\text{Nd}, \text{Sr})\text{NiO}_2$, *Phys. Rev. Lett.* **125**, 077003 (2020).
- [85] Y. Nomura, M. Hirayama, T. Tadano, Y. Yoshimoto, K. Nakamura, and R. Arita, Formation of a two-dimensional single-component correlated electron system and band engineering in the nickelate superconductor NdNiO_2 , *Phys. Rev. B* **100**, 205138 (2019).
- [86] L. Wang, Z. F. Yang, K. P. Koirala, M. E. Bowden, J. W. Freeland, P. V. Sushko, C.-T. Kuo, S. A. Chambers, C. M. Wang, B. Jalan, and Y. G. Du, Interfacial charge transfer and its impact on transport properties of $\text{LaNiO}_3/\text{LaFeO}_3$ superlattices, *Sci. Adv.* **10**, eadq6687 (2024).
- [87] F. Yao, L. F. Zhang, J. L. Meng, X. J. Liu, X. Zhang, W. W. Zhang, J. Meng, and H. J. Zhang, Tuning charge transfer in the $\text{LaTiO}_3/\text{RO}/\text{LaNiO}_3$ (R = rare-earth) superlattices by the rare-earth oxides interfaces from a first-principles calculation, *J. Appl. Phys.* **123**, 115304 (2018).
- [88] Y. K. Weng, J.-J. Zhang, B. Gao, and S. Dong, $(\text{LaTiO}_3)_n/(\text{LaVO}_3)_n$ as a model system for unconventional charge transfer and polar metallicity, *Phys. Rev. B* **95**, 155117 (2017).
- [89] M. Kitatani, L. Si, O. Janson, R. Arita, Z. C. Zhong, and K. Held, Nickelate superconductors—a renaissance of the one-band Hubbard model, *npj Quantum Mater.* **5**, 59 (2020).
- [90] X. Ding, Y. Fan, X. X. Wang, C. H. Li, Z. T. An, J. H. Ye, S. L. Tang, M. Y. N. Lei, X. T. Sun, N. Guo *et al.*, Cuprate-like

- electronic structures in infinite-layer nickelates with substantial hole dopings, *Natl. Sci. Rev.* **11**, nwae194 (2024).
- [91] W. J. Sun, Z. C. Jiang, C. L. Xia, B. Hao, S. J. Yan, M. S. Wang, Y. Y. Li, H. Q. Liu, J. Y. Ding, J. Y. Liu *et al.*, Electronic structure of superconducting infinite-layer lanthanum nickelates, *Sci. Adv.* **11**, eadr5116 (2025).
- [92] K. H. Lee, B. Y. Wang, M. Osada, B. H. Goodge, T. C. Wang, Y. H. Lee, S. Harvey, W. J. Kim, Y. J. Yu, C. Murthy *et al.*, Linear-in-temperature resistivity for optimally superconducting (Nd, Sr)NiO₂, *Nature (London)* **619**, 288 (2023).
- [93] S. L. E. Chow, Z. Y. Luo, and A. Ariando, Bulk superconductivity near 40 K in hole-doped SmNiO₂ at ambient pressure, *Nature (London)* **642**, 58 (2025).
- [94] The strong overlap between La-4*f* and-5*d* orbitals around 2 eV complicates the construction of La-5*d* + Ni-3*d* Wannier functions, as neglecting La-4*f* states requires a broad energy window and more DFT Bloch bands, hindering high-quality of the projection.
- [95] M. Kitatani, L. Si, P. Worm, J. M. Tomczak, R. Arita, and K. Held, Optimizing superconductivity: From cuprates via nickelates to palladates, *Phys. Rev. Lett.* **130**, 166002 (2023).
- [96] M. Hirayama, T. Tadano, Y. Nomura, and R. Arita, Materials design of dynamically stable *d*⁹ layered nickelates, *Phys. Rev. B* **101**, 075107 (2020).
- [97] B. G. Csire and J. F. Annett, Nonunitary triplet pairing in the noncentrosymmetric superconductor LaNiC₂, *Eur. Phys. J. B* **91**, 217 (2018).
- [98] G. Campi, A. Alimenti, G. Logvenov, G. A. Smith, F. Balakirev, S.-E. Lee, L. Balicas, E. Silva, G. A. Ummarino, G. Midei, A. Perali, A. Valletta, and A. Bianconi, Upper critical magnetic field and multiband superconductivity in artificial high-*T*_c superlattices of nano quantum wells, *Phys. Rev. Mater.* **9**, 074204 (2025).
- [99] Novel Materials Discovery (NOMAD) repository, [10.17172/NOMAD/2026.01.26-2](https://doi.org/10.17172/NOMAD/2026.01.26-2).