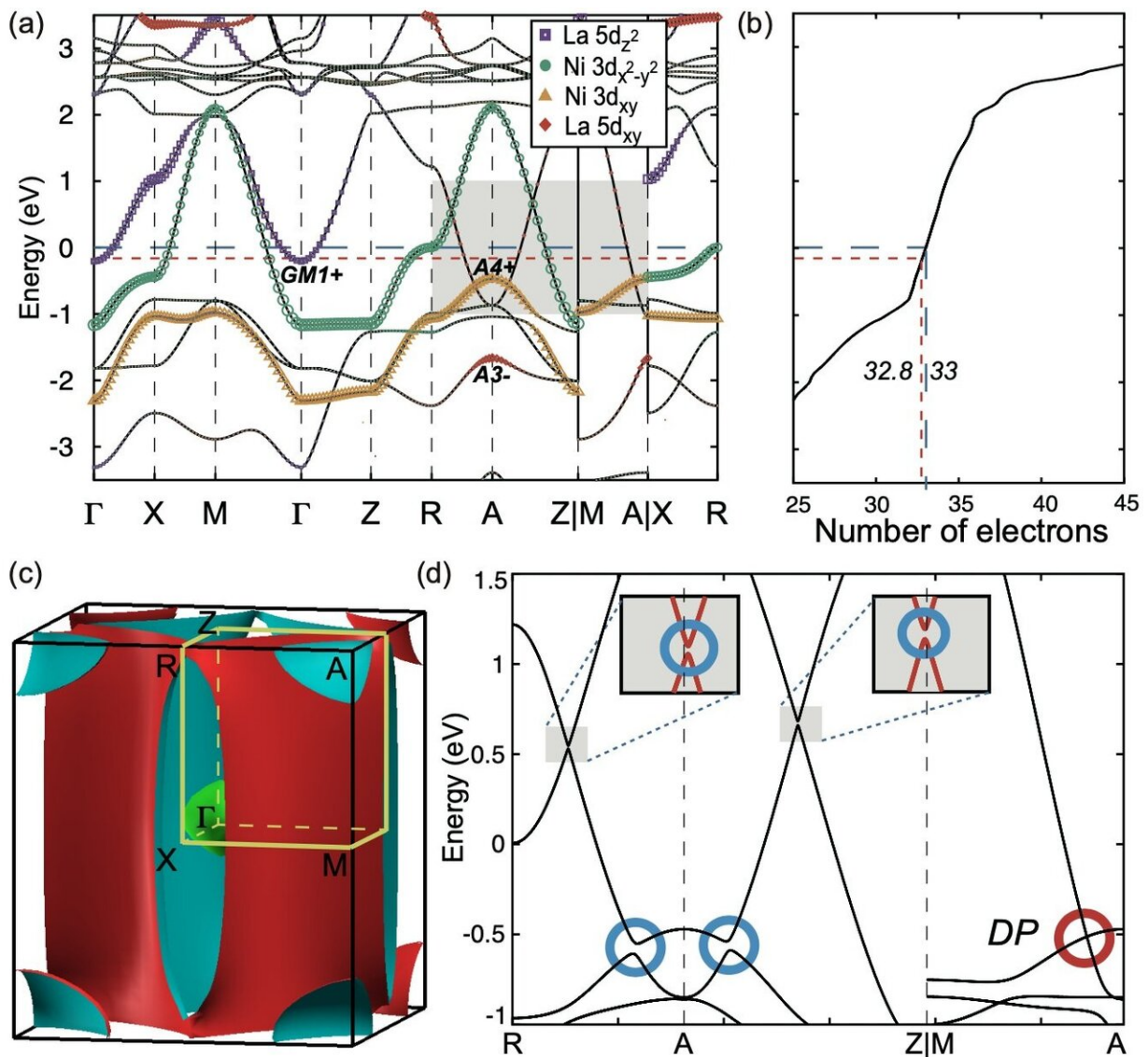


Progress in electronic structure and topology in nickelates superconductors

November 25 2020



(a) The band structure of LaNiO₂ without SOC. The weights of different

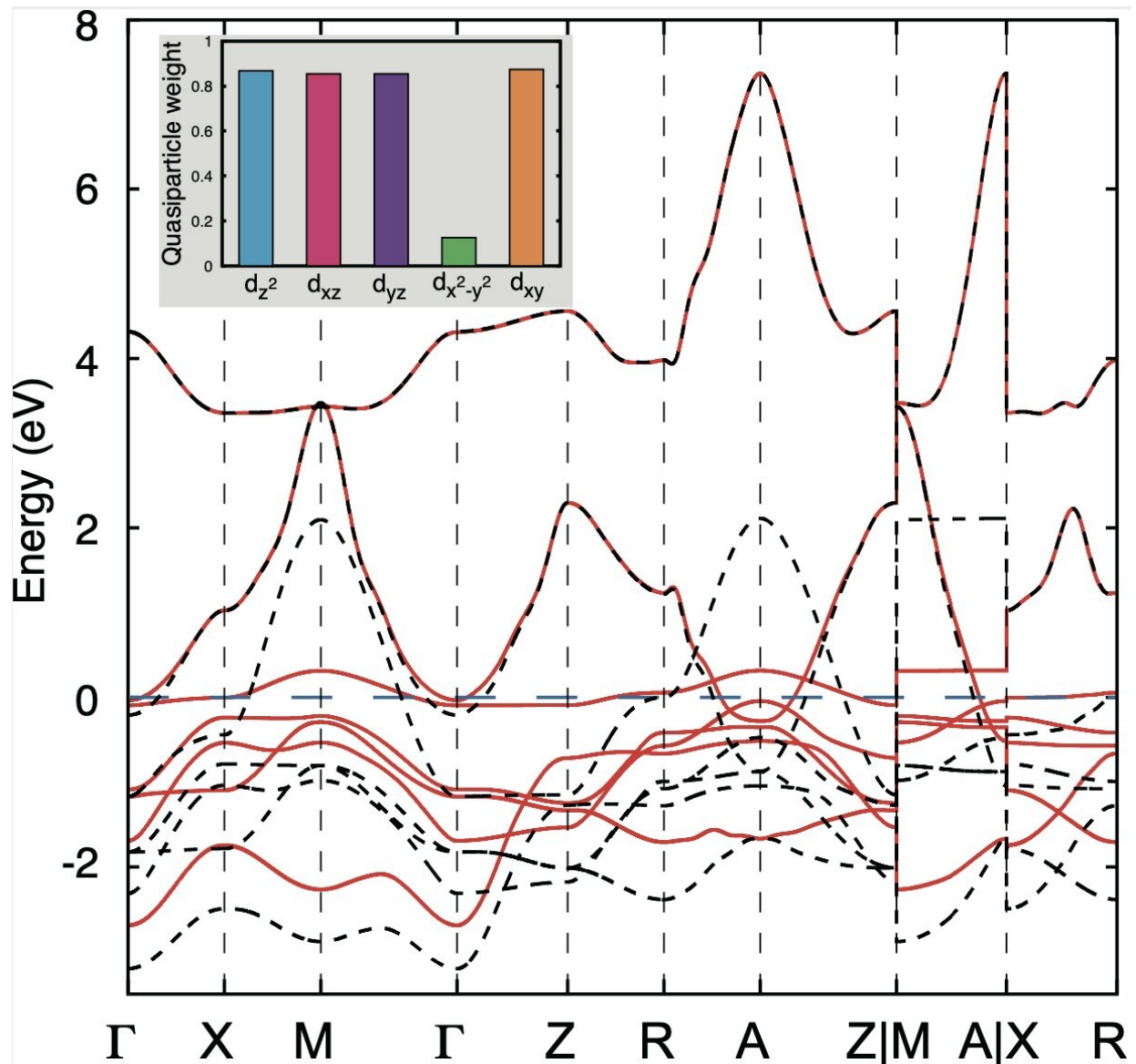
orbitals are represented by different colors. (b) The total number of electrons as a function of chemical potential. (c) The Fermi surface of LaNiO_2 . (d) The band structure with SOC in the shadowed area of (a), the crossings are gapped except the Dirac points along M-A. Credit: ©Science China Press

The discovery of high T_c superconductivity in cuprates attracts people to explore superconductivity in nickelates, whose crystal structures are similar to cuprates. Recently, Danfeng Li et al. at Stanford University published an article in *Nature*, reporting the observed superconductivity in hole-doped nickelates $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$. Different from cuprates, the parent compound NdNiO_2 does not preserve long range magnetic order, which was thought to be responsible for superconductivity in copper oxides. Besides, the ground state of NdNiO_2 is metallic. The comment article in *Nature* noted that Li's work could become a game changer for our understanding of superconductivity in cuprates and cuprate-like systems, perhaps leading to new high-temperature superconductors.

In order to understand the mechanism of nickelates superconductors, scientists at the Institute of Physics, Chinese Academy of Science made a careful analysis on the parent compound NdNiO_2 , including its [electronic band structure](#), orbital characteristics, Fermi surfaces and band topology by using first-principles calculations and Gutzwiller variational method. The results show that the electron Fermi pockets are contributed by $\text{Ni-3d}_{x^2-y^2}$ orbitals, while hole pockets consist of $\text{Nd-5d}_{3z^2-r^2}$ and Nd-5d_{xy} orbitals. By analyzing elementary band representation in the theory of topological quantum chemistry, the authors found that a two-band model can be constructed to reproduce all bands around Fermi level.

The two bands originate from two orbitals, including one $\text{Ni-3d}_{x^2-y^2}$ orbital and one s-like pseudo-orbital located on the vacancy of oxygen

atoms. Besides, the authors found that band inversion happens between Ni- $3d_{xy}$ states and conduction bands, resulting in a pair of Dirac points along M-A in the Brillouin zone. In addition, to take the correlation effects of Ni 3d electrons into consideration, the authors performed the DFT + Gutzwiller calculation. The results show that the half occupied $3d_{x^2-y^2}$ orbital have the smallest quasiparticle weight (about 0.12); namely, the $3d_{x^2-y^2}$ band width after renormalization is about 1/8 of DFT results. On the other hand, the Dirac points along M-A high symmetry line become closer to the Fermi level due to the band renormalization. In this work authors calculated the electronic structure, discussed topological properties and constructed a two-band model. These results will help people for the study of topology and [superconductivity](#) in nickelates.



The band structure of non-interacting tight-binding model is plotted in black dashed lines, while the DFT+Gutzwiller bands are plotted in red solid lines. The inset shows the quasiparticle weights of five 3d orbitals. Credit: ©Science China Press

More information: Jiacheng Gao et al, Electronic structures and

topological properties in nickelates $L_n + 1Ni_nO_{2n+2}$, *National Science Review* (2020). [DOI: 10.1093/nsr/nwaa218](https://doi.org/10.1093/nsr/nwaa218)

Provided by Science China Press

Citation: Progress in electronic structure and topology in nickelates superconductors (2020, November 25) retrieved 25 April 2024 from <https://phys.org/news/2020-11-electronic-topology-nickelates-superconductors.html>

This document is subject to copyright. Apart from any fair dealing for the purpose of private study or research, no part may be reproduced without the written permission. The content is provided for information purposes only.