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Nickelate superconductors get 'hotter'

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For more than three decades, the quest for superconductivity in nickel oxides, also known as nickelates, has symbolized the unwavering dedication in search for an analogy to the Nobel Prize-winning high-temperature superconducting copper oxides, or cuprates [1]. This long-cherished aspiration has finally been achieved by the discovery of superconductivity in a topochemically [2] prepared infinite-layer thin-film nickelate, $Nd_{1-x}Sr_xNiO_2$ [3]. Of particular significance is the unique Ni^{1+} valence state, which closely resembles the $3d^9$ electronic configuration—a plausible common feature shared with cuprates. In a relatively short span of time, an extended material family possessing unusual reduced nickel valences was further discovered [4]. These findings, together with a host of intriguing properties [5] for which electron correlations may play an important role, have ushered a new era in the study of unconventional superconductivity.

A subtle yet crucial distinction between nickelates and cuprates lies in their electronic configurations. Unlike cuprates, where a charge-transfer scenario prevails, nickelates with Ni^{1+} exhibit a Mott-Hubbard orbital alignment. This distinction affects the covalent hybridization between O 2p and transition-metal 3d orbitals, which is central to cuprates and vital for the formation of the Zhang-Rice singlet [6]. In nickelate compounds, this hybridization is significantly reduced. Factors that may contribute to the generally lower superconducting transition temperature (T_c) [3,5], even under high pressures [7], have been extensively discussed. Nickelate compounds featuring larger electronic bandwidth and stronger correlations between Ni 3d and O 2p bands hold greater promise as candidates for high-temperature superconductors.

Writing in *Nature* [8], scientists from Wang's group at Sun Yat-sen University in China reported the signature of superconductivity at temperatures as high as near 80 K in a single-crystalline bilayer Ruddlesden-Popper nickelate, $La_3Ni_2O_7$, under high pressures between 14–43.5 GPa. This discovery is phenomenal as the T_c surpasses the record value achieved in thin-film infinite-layer nickelates [5,7], marking the second category of unconventional superconductors with T_c above the liquid nitrogen boiling temperature (the other category includes some members of cuprate family).

Unlike that in the infinite-layer phase, the Ni cations in $La_3Ni_2O_7$ single crystals have an average valence of +2.5: the presence of two distinctive Ni sites with varied electron counts. In particular, the $3d_{x^2-y^2}$ and $3d_{z^2}$ bands contribute to the electronic states near Fermi level with strong O 2p orbital characteristics, and a gap opening within the half-filled $3d_{z^2}$ manifolds due to a strong orbital hybridization. The authors propose that, upon the application of pressure, the $3d_{z^2}$ bonding 'flat bands' are further lifted in energy and get 'hole-doped', leading to the metallization of the $3d_{z^2}$ σ-bonds, essential for superconductivity. What is intriguing is that the emergence of the high-T_c superconducting state is associated with a structural phase transition from a low-pressure orthorhombic *Amam* phase to a high-pressure orthorhombic *Fmmm* phase, in which the out-of-plane Ni–O–Ni bonds straighten. Evidently, the

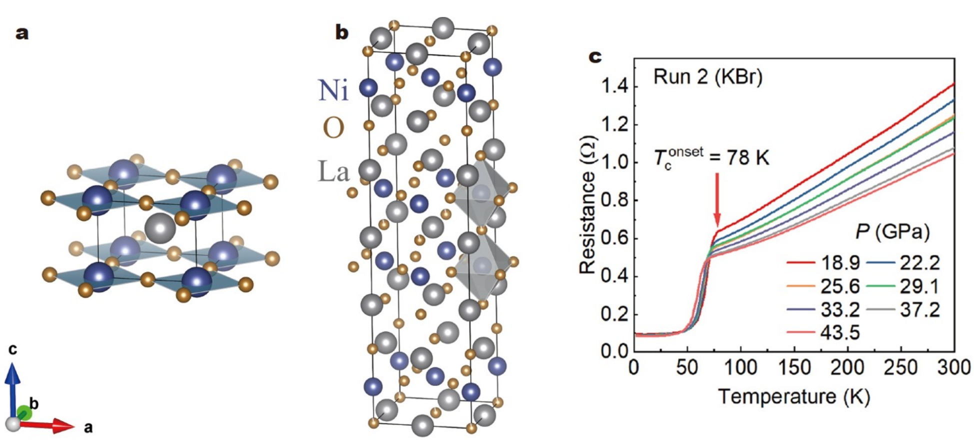

Figure 1 Crystal structures of (a) the infinite-layer nickelate, $LaNiO_2$, and (b) the bilayer nickelate, $La_3Ni_2O_7$; (c) resistance of $La_3Ni_2O_7$ *versus* temperature under different pressures. Reprinted with permission from Ref. [8]. Copyright 2023, Nature Publishing Group.

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inter-layer coupling of the $3d_{z^2}$ orbitals, along with the newly stabilized crystal structure and the pronounced involvement of the O 2p orbitals, plays a predominant role in the emergence of superconductivity. These important factors are anticipated to give rise to distinctive features as compared with cuprates, including magnetic structures, therefore raising important questions regarding the origin of high-temperature superconductivity.

Clearly, the momentum in searching for ever-better superconductors and the recent reignited focus on nickelate compounds have motivated this fascinating discovery. As attested by independent research groups [9,10], this discovery will open a flourishing arena for the study of high-temperature superconductors and has rekindled the enthusiasm of the research community in tackling fundamental challenges in understanding high-temperature superconductivity. This remarkable achievement serves as another vivid illustration of how dedicated efforts in material synthesis can yield groundbreaking results, akin to the surprising revelation of cuprate superconductivity from ceramic materials several decades ago. With this latest discovery, the stage is set for an exciting journey of exploration and innovation in the realm of high-temperature superconductivity.

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