# Finding superconductivity in nickelates

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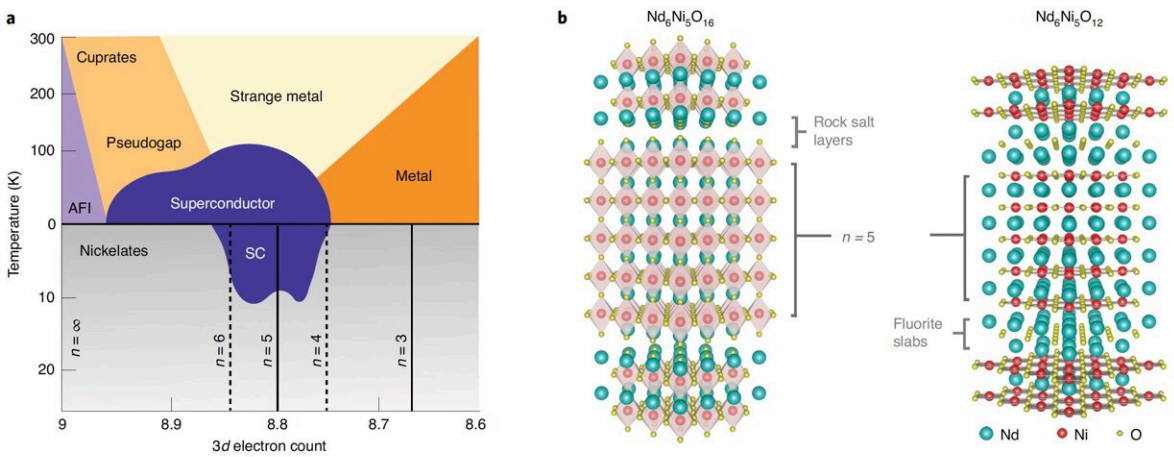


Electronic phase diagram and structural description of the layered nickelates. A: Schematic phase diagram for the electronic phases of the cuprates (top) and nickelates (bottom). B: Crystal structures of the quintuple-layer nickelates in the Nd6Ni5O16 Ruddlesden–Popper phase (left) and Nd6Ni5O12 reduced square-planar phase (right), depicted at the same scale. Credit: Botana et al.

The study of superconductivity is littered with disappointments, dead ends, and serendipitous discoveries, according to Antia Botana, professor of physics at Arizona State University.

"As theorists, we generally fail in predicting new superconductors," she said.

However, in 2021, she experienced the highlight of her early career. Working with experimentalist Julia Mundy at Harvard University, she discovered a new superconducting material—a quintuple-layer nickelate. They reported their findings in Nature Materials in September 2021.

"It was one of the best moments of my life," Botana recalled. "I was flying back from Spain, and I received a message from my collaborator Julia Mundy during my layover. When I saw the resistivity drop to zero—there's nothing better than that."

Botana was chosen as a 2022 Sloan Research Fellow. Her research is supported by a CAREER award from the National Science Foundation (NSF).

"Prof. Botana is one of the most influential theorists in the field of unconventional superconductivity, particularly in layered nickelates that have received tremendous attention from the materials and condensed matter physics communities," said Serdar Ogut, Program Director in the Division of Materials Research at the National Science Foundation. "I expect that her pioneering theoretical studies, in collaboration with leading experimentalists in the U.S., will continue to push the boundaries, result in the discovery of new superconducting materials, and uncover fundamental mechanisms that could one day pave the way to room temperature superconductivity."

Superconductivity is a phenomenon that occurs when electrons form pairs rather than traveling in isolation, repulsing all magnetism, and allowing electrons to travel without losing energy. Developing room-temperature superconductors would allow loss-free electricity transmission and faster, cheaper quantum computers. Studying these materials is the domain of condensed matter theory.

"We try to understand what are called quantum materials—materials

where everything classical that we learned in our undergraduate studies falls apart and no one understands why they do the fun things they do," Botana joked.

She began investigating nickelates, largely, to better understand cuprates—copper-oxide based superconductors first discovered in 1986. Thirty years on, the mechanism that produces superconductivity in these materials is still hotly contested.

Botana approaches the problem by looking at materials that look like cuprates. "Copper and nickel are right next to each other on the periodic table," she said. "This was an obvious thing to do, so people had been looking at nickelates for a long time without success."

But then, in 2019, a team from Stanford discovered superconductivity in a nickelate, albeit one that had been "doped," or chemically-altered to improve its electronic characteristics. "The material that they found in 2019 is part of a larger family, which is what we want, because it lets us do comparisons to cuprates in a better way," she said.

Botana's discovery in 2021 built on that foundation, using a form of undoped nickelate with a unique, square-planar, layered structure. She decided to investigate this specific form of nickelate—a rare-earth, quintuple-layer, square-planar nickelate—based on intuition.

"Having played with many different materials for years, it's the type of intuition that people who study electronic structure develop," she said. "I have seen that over the years with my mentors."

Identifying another form of superconducting nickelate lets researchers tease out similarities and differences among nickelates, and between nickelates and cuprates. So far, the more nickelates that are studied, the more like cuprates they look.

"The phase diagram seems quite similar. The electron pairing mechanism seems to be the same," Botana says, "but this is a question yet to be settled."

Conventional superconductors exhibit s-wave pairing—electrons can pair in any direction and can sit on top of each other, so the wave is a sphere. Nickelates, on the other hand, likely display d-wave pairing, meaning that the cloudlike quantum wave that describes the paired electrons is shaped like a four-leaf clover. Another key difference is how strongly oxygen and transition metals overlap in these materials. Cuprates exhibit a large "super-exchange"—the material trades electrons in copper atoms through a pathway that contains oxygen, rather than directly.

"We think that may be one of the factors that governs superconductivity and causes the lower critical temperature of the nickelates," she said. "We can look for ways of optimizing that characteristic."

Botana and colleagues Kwan-Woo Lee, Michael R. Norman, Victor Pardo, Warren E. Pickett described some of these differences in a review article for *Frontiers in Physics* in February 2022.

## Searching for root causes of superconductivity

Writing in *Physical Review X* in March 2022, Botana and collaborators from the Brookhaven National Laboratory and Argonne National Labs delved deeper into the role of oxygen states in the low-valence nickelate $La_4Ni_3O_8$. Using computational and experimental methods, they compared the material to a prototypical cuprate with a similar electron filling. The work was unique in that it directly measured the energy of the nickel-oxygen hybridized states.

They found that despite requiring more energy to transfer charges,

nickelates retained a sizable capacity for superexchange. They conclude that both the "Coulomb interactions" (the attraction or repulsion of particles or objects because of their electric charge) and charge-transfer processes need to be considered when interpreting the properties of nickelates.

The quantum phenomena that Botana studies occur at the smallest scales known and can only be probed obliquely by physical experiment (as in the *Physical Review X* paper). Botana uses computational simulations to make predictions, help interpret experiments, and deduce the behavior and dynamics of materials like infinite-layer nickelate.

Her research uses Density Functional Theory, or DFT—a means of computationally solving the Schrödinger equation that describes the wave function of a quantum-mechanical system—as well as a newer, more precise offshoot known as dynamical mean field theory that can treat electrons that are strongly correlated.

To conduct her research, Botana uses the Stampede2 supercomputer of the Texas Advanced Computing Center (TACC)—the second fastest at any university in the U.S.—as well as machines at Arizona State University. Even on the fastest supercomputers in the world, studying quantum materials is no simple matter.

"If I see a problem with too many atoms, I say, 'I can't study that,'" Botana said. "Twenty years ago, a few atoms might have looked like too much." But more powerful supercomputers are allowing physicists to study larger, more complicated systems—like nickelates—and add tools, like dynamical mean field theory, that can better capture quantum behavior.

Despite living in a Golden Age of Discovery, the field of condensed matter physics still doesn't have the reputation it deserves, Botana says.

"Your phone or computer would not be possible without research in condensed matter physics—from the screen, to the battery, to the little camera. It's important for the public to understand that even if it's fundamental research, and even if the researchers don't know how it will be used later, this type of research in materials is critical."

**More information:** Y. Shen et al, Role of Oxygen States in the Low Valence Nickelate La4Ni3O8, *Physical Review X*, (2022). DOI: 10.1103/PhysRevX.12.011055

Antia S. Botana et al, Low Valence Nickelates: Launching the Nickel Age of Superconductivity, *Frontiers in Physics*, (2022). DOI: 10.3389/fphy.2021.813532

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