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How to make a cuprate Fermi surface out of a nickelate heterostructure

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Chaloupka and Khaliullin had the idea that it might be possible to make Ni³⁺-based high-temperature superconductors by sandwiching NiO₂ layers between insulating layers through heterostructuring.² Provided that spin-, charge-, and orbital ordering can be avoided, the confinement should make it possible to empty the Ni $3z^2 - 1$ band, thus leaving the conduction electron in the Ni $x^2 - y^2$ band. Fabrication of such heterostructures are now being pursued in many laboratories. We³ have attempted to give theoretical guidance by performing calculations for numerous heterostructures using the local density-approximation in combination with static (LDA+U) and dynamical (LDA+DMFT) mean-field theory. We show how confinement together with electronic correlations can lead to a single-sheet Fermi surface with a shape like that of the cuprate superconductors with the highest transition temperatures; the Ni $3z^2 - 1$ Wannier orbital now plays the role of the axial, Cu $4s$ -like orbital in the cuprates.⁴ Since also strong antiferromagnetic fluctuations are present, the low-energy electronic and spin excitations should resemble those of high-temperature cuprate superconductors. Chemical modification of the insulating layers should make it possible to avoid spin-, charge-, and orbital ordering.

²J. Chaloupka and G. Khaliullin, Phys. Rev. Lett. **100**, 016404 (2008).

³P. Hansmann, Xiaoping Yang, A. Tosci, G. Khaliullin, O.K. Andersen, and K. Held, arXiv: 0807.0407.

⁴E. Pavarini, I. Dasgupta, T. Saha-Dasgupta, O. Jepsen, and O. K. Andersen, Phys. Rev. Lett. **87**, 047003 (2001).

¹With Xiaoping Yang, P. Hansmann, A. Tosci, G. Khaliullin, and K. Held