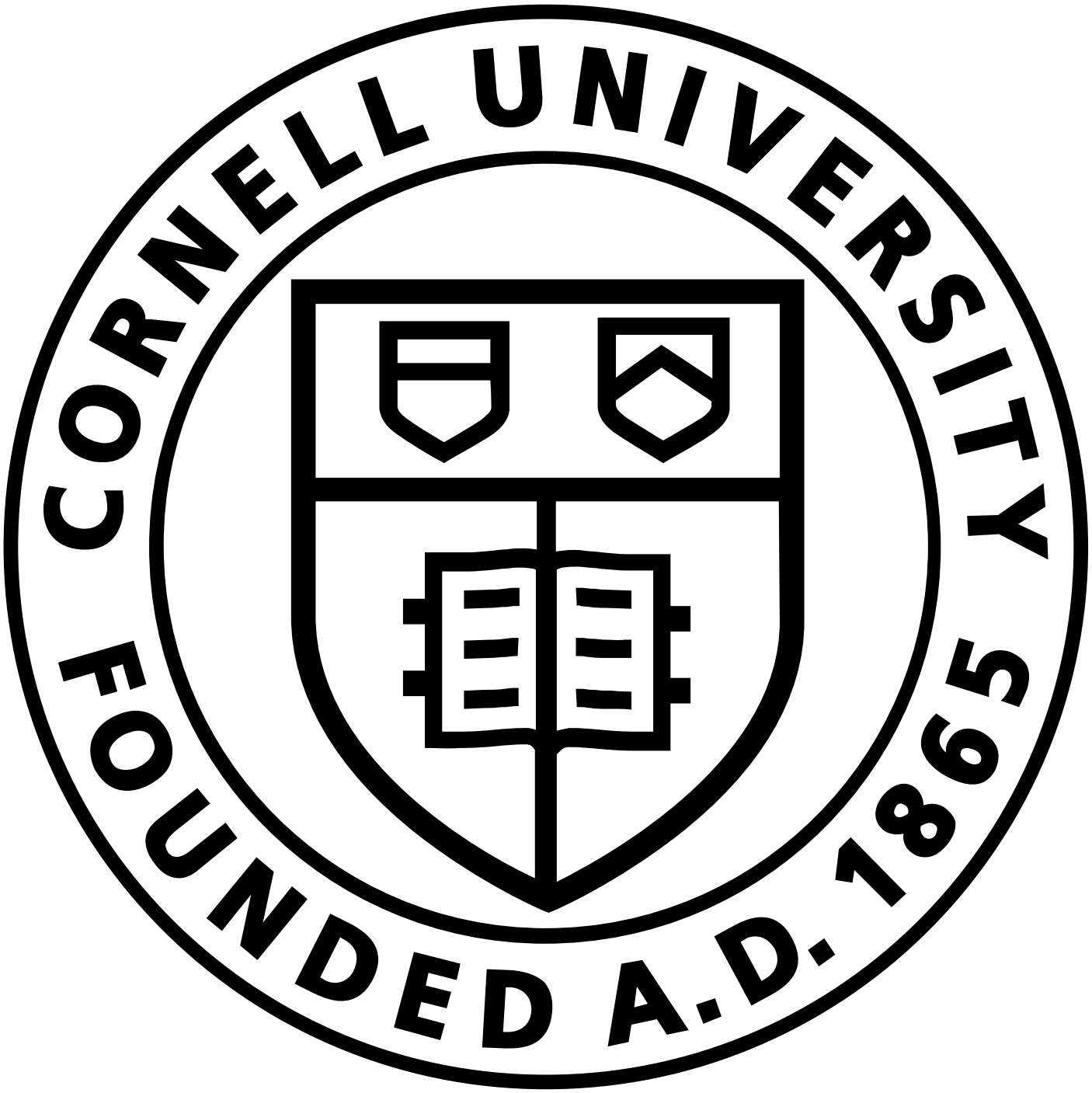

Condensed Matter > Superconductivity

arXiv:2307.16892 (cond-mat)

[Submitted on 31 Jul 2023]

Origin of correlated isolated flat bands in copper-substituted lead phosphate apatite

Sinéad M. Griffin

A recent report of room temperature superconductivity at ambient pressure in Cu-substituted apatite (`LK99') has invigorated interest in the understanding of what materials and mechanisms can allow for high-temperature superconductivity. Here I perform density functional theory calculations on Cu-substituted lead phosphate apatite, identifying correlated isolated flat bands at the Fermi level, a common signature of high transition temperatures in already established families of superconductors. I elucidate the origins of these isolated bands as arising from a structural distortion induced by the Cu ions and a chiral charge density wave from the Pb lone pairs. These results suggest that a minimal two-band model can encompass much of the low-energy physics in this system. Finally, I discuss the implications of my results on possible superconductivity in Cu-doped apatite

Subjects: **Superconductivity (cond-mat.supr-con)**; Materials Science (cond-mat.mtrl-sci); Strongly Correlated Electrons (cond-mat.str-el)

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