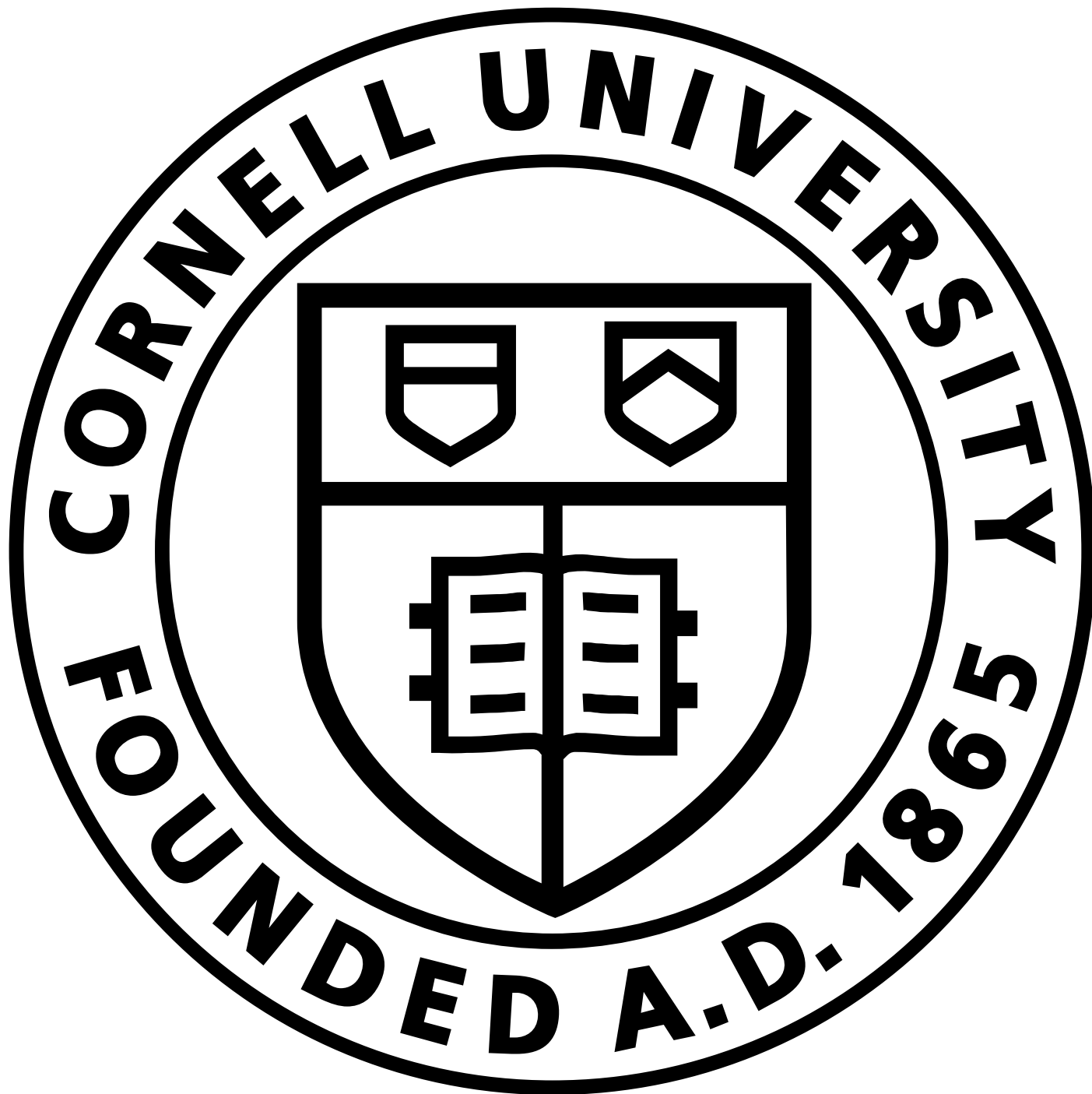


[Skip to main content](#)

> [cond-mat](#) > arXiv:2307.16892



Search...

GO

## quick links

- [Login](#)
- [Help Pages](#)
- [About](#)

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](#)


[Download PDF](#)

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)

Cite as: [arXiv:2307.16892](#) [cond-mat.supr-con]  
(or [arXiv:2307.16892v1](#) [cond-mat.supr-con] for this version)

<https://doi.org/10.48550/arXiv.2307.16892>

 Focus to learn more

arXiv-issued DOI via DataCite

## Submission history

From: Sinéad Griffin Dr. [[view email](#)]

[v1] Mon, 31 Jul 2023 17:58:17 UTC (7,923 KB)

Bibliographic Tools

## Bibliographic and Citation Tools

Bibliographic Explorer Toggle

Bibliographic Explorer ([What is the Explorer?](#))

Litmaps Toggle

Litmaps ([What is Litmaps?](#))

scite.ai Toggle

scite Smart Citations ([What are Smart Citations?](#))

Code, Data, Media

## Code, Data and Media Associated with this Article

Links to Code Toggle

CatalyzeX Code Finder for Papers ([What is CatalyzeX?](#))

DagsHub Toggle

DagsHub ([What is DagsHub?](#))

Links to Code Toggle

Papers with Code ([What is Papers with Code?](#))

ScienceCast Toggle

ScienceCast ([What is ScienceCast?](#))

Demos

## Demos

Replicate Toggle

Replicate ([What is Replicate?](#))

Spaces Toggle

Hugging Face Spaces ([What is Spaces?](#))

Related Papers

## Recommenders and Search Tools

Link to Influence Flower

Influence Flower ([What are Influence Flowers?](#))

Connected Papers Toggle

Connected Papers ([What is Connected Papers?](#))

Core recommender toggle

CORE Recommender ([What is CORE?](#))

IArxiv recommender toggle

IArxiv Recommender ([What is IArxiv?](#))

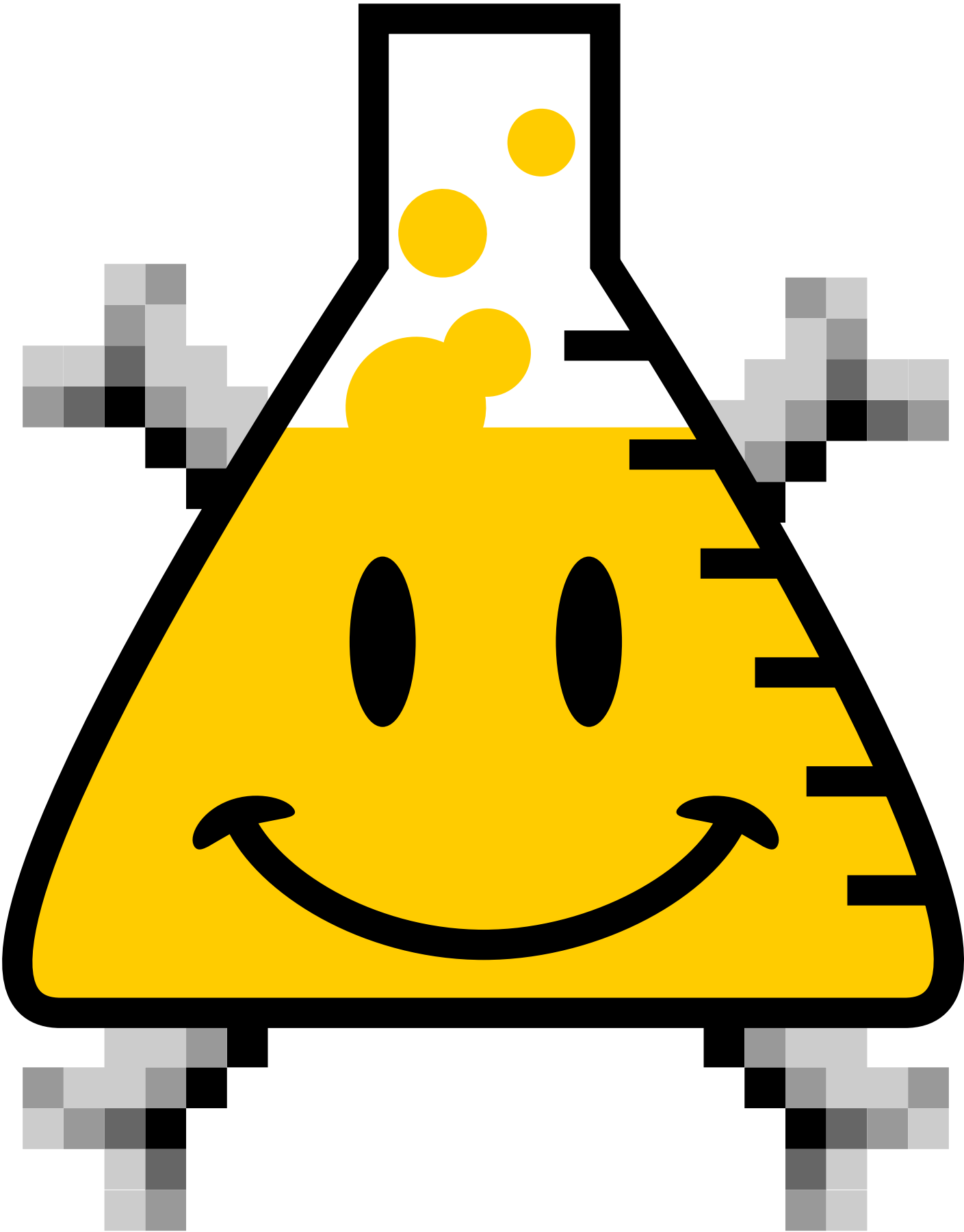
About arXivLabs

## arXivLabs: experimental projects with community collaborators

arXivLabs is a framework that allows collaborators to develop and share new arXiv features directly on our website.

Both individuals and organizations that work with arXivLabs have embraced and accepted our values of openness, community, excellence, and user data privacy. arXiv is committed to these values and only works with partners that adhere to them.

Have an idea for a project that will add value for arXiv's community? [Learn more about arXivLabs.](#)



[Which authors of this paper are endorsers?](#) | [Disable MathJax](#) ([What is MathJax?](#))