

Two room-temperature superconductivity claims in 2023: Separating fact from fiction

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In 2023, two experimental claims of room-temperature superconductivity shocked the world. The first claimed to show near-ambient superconductivity in lutetium-hydride compounds coinciding with drastic colour changes of the samples from blue to pink to red [1]. We present a full microscopic theory of colour in lutetium hydride, revealing that hydrogen-deficient LuH_2 is the only phase which exhibits colour changes under pressure consistent with experimental reports, with a sequence blue-violet-pink-red-orange (Fig. 1) [2]. In addition, we find *no* phonon-mediated superconductivity near room temperature in the claimed pink phase.

The second claim concerns “LK99” [3], a copper-doped lead apatite compound which has motivated numerous contradictory theoretical reports. Puzzlingly, previous theoretical works claimed that experimentally reported structures of both the parent and copper-doped lead apatite are dynamically unstable. By pioneering the inclusion of anharmonic phonon-phonon interactions, we show that both compounds are dynamically stable at room temperature, consistent with the experimental reports (Fig. 2a) [4]. We resolve all existing inconsistencies about the dynamical stability of the LK99 compound by clarifying the role of volume and electronic correlation strength. Furthermore, we demonstrate it is *not* a superconductor but instead a strongly correlated Mott insulator whose phenomenology differs from that of d^9 cuprate superconductors by performing comprehensive DFT+DMFT calculations in Hubbard U-J parameter spaces (Fig. 2b) [5].

References

- [1] N. Dasenbrock-Gammon *et al.*, Nature **615**, 244 (2023)
- [2] S.-W. Kim *et al.*, Nature Communications **14**, 7360 (2023)
- [3] S. Lee *et al.*, arXiv:2307.12037 (2023)
- [4] S.-W. Kim *et al.*, npj Computational Materials **10**, 16 (2024)
- [5] S.-W. Kim *et al.*, in preparation

Figures

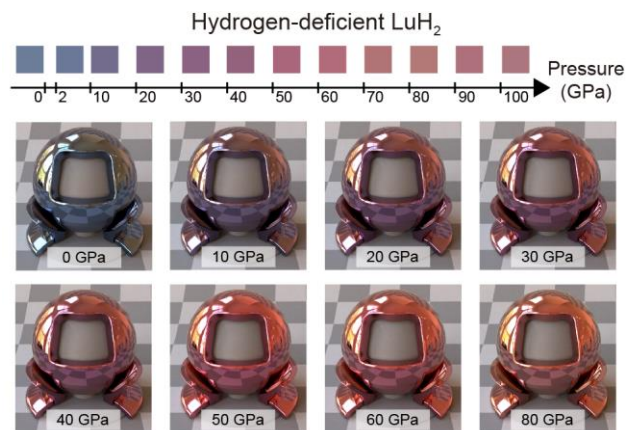


Figure 1: Colour and photorealistic rendering of hydrogen-deficient LuH_2 as a function of pressure.

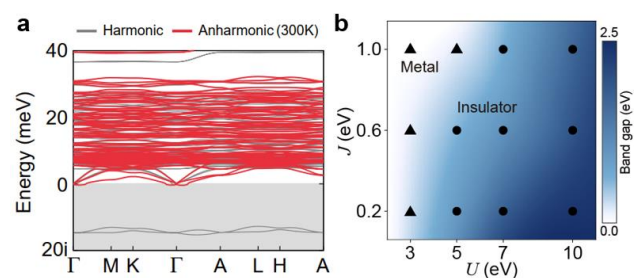


Figure 2: (a) Harmonic and anharmonic phonon dispersions and (b) Hubbard U-J phase diagram of the LK99 compound.

Acknowledgements

The following collaborators have contributed to some or all of these works: Kang Wang, Siyu Chen, Lewis J. Conway, Ion Errea, G. Lucian Pascut, Kristjan Haule, Chris J. Pickard, and Bartomeu Monserrat.