we would like to present back-to-back with the following contribution:
Paula Giraldo-Gallo et al., "Fermiology of the low carrier density superconductor Tl-doped PbTe, and its non-superconducting analog, Na-doped PbTe"
Thank you very much!

Abstract Submitted

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First-principles Fermi surface of doped PbTe BORIS SANGIORGIO, Materials Theory, ETH Zurich, PAULA GIRALDO-GALLO, Stanford University, MICHAEL FECHNER, Materials Theory, ETH Zurich, IAN FISHER, Stanford University, NICOLA SPALDIN, Materials Theory, ETH Zurich — PbTe is a narrow-gap semiconductor and one of the leading thermoelectric materials above room temperature. When doped with Tl atoms an unusual superconducting state is observed that persists to $\sim$ 1.5 K, 1 order of magnitude higher than in non-Tl-based systems. The nature of the superconductivity is not well understood, with a charge Kondo effect suggested as the underlying pairing mechanism. In this study we investigate the electronic properties - in particular the Fermi surface - of doped PbTe using first-principles calculations. First, we use the rigid band approximation to compute de Haas-van Alphen frequencies and compare them to recent quantum-oscillations experiments on Na- and Tl-doped PbTe. With the use of supercells we confirm the usefulness of the rigid-band approximation for Na impurities. In contrast, we find that the electronic properties are strongly affected by Tl impurities: a narrow "impurity band" (originating from hybridization between Tl s and Te p states) is found at the Fermi energy suggesting an electronic instability, such as a charge disproportionation, which is likely relevant for the superconductivity.

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