Out of phase multiband charge modulations in 2H-NbSe$_2$

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The charge density wave (CDW) state is an electronic order where the charge density develops a spatial modulation concomitantly to a periodic distortion of the atomic lattice. The new periodicity leads to the reorganization of the electronic bands of the parent compound through their back-folding on the new Brillouin-zone. Although a gap in the quasi-particle spectrum should open at all the crossings of the folded bands, previous studies only focused on the primary CDW gap around the Fermi-level. The existence of secondary gaps and associated charge modulations in charge ordered materials remains largely unexplored.

We show that by combining energy-dependent scanning tunnelling microscopy (STM) topography with a simple model of the charge modulations and a self-consistent calculation of the CDW gap, we find evidence for a multiband CDW in 2H-NbSe$_2$ [1]. This CDW not only involves the opening of a gap on the inner band around the K-point but also on the outer band. This leads to spatially out of phase charge modulations from electrons on these two bands, which we detect through a characteristic energy dependence of the CDW contrast in topographic STM images.