Evidence of band folding in the charge density wave of 4Hb-TaSe2

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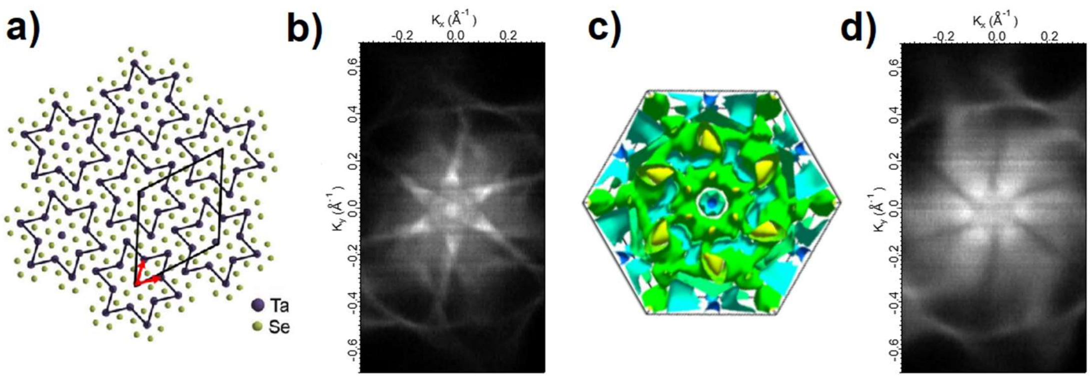
Charge density wave (CDW) materials are attracting much interest in the scientific community due to fascinating phenomena associated with their metal to insulator transitions [1]. Layered structures of the transition metal dichalcogenide (TMD) tantalum diselenide, TaSe2, display a rich polymorphism, with all the different crystal structures - and in particular the 2H, 1T and 4Hb - exhibiting CDWs. 2H and 1T CDWs are characterized by a 3x3 and √13x√13 lattice reconstruction, respectively. The latter corresponds to a star-like cluster structure rotated by 13.9° in the ab crystallographic plane (Fig. 1a). Both systems have been extensively investigated by ARPES [2-4]. Nevertheless, in the case of the 1T, a clear signature of CDW completely reconstructed bands appears hidden within broad band features, possibly due to dimerization between layers or other interlayer interactions [5].

In this work, we present the results of a combined ARPES experiments and theoretical DFT investigation, addressing the CDWs in 4Hb-TaSe2 crystals, and focusing in particular on the surface termination with the 1T layer. As shown in Fig. 1b and c, the ARPES Fermi-map displays a star-shaped Fermi surface close to the $\bar{\Gamma}$ point, with the orientation of the tips of the star consistent with the 13.9°-rotation and in agreement with theory. Moreover, the map taken at –50 meV below Fermi (Fig. 1d) also highlights a certain degree of chirality [6]. This is the first time that the folded band structure of the √13x√13 CDW has been recorded with such details, demonstrating how the 4Hb structure offers an opportunity to study the star cluster CDW in the T layer and its chirality in a configuration close to the 2D limit.



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