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Charge Density Waves in ZrTe3: the fate of nesting in real 3D materials

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Among the materials hosting Charge Density Wave (CDW) phases, transition metal tri-chalcogenides have attracted considerable attention thanks to their quasi-one-dimensional (1D) nature. ZrTe3 is of particular interest because its Fermi surface comprises both a 3D hole like pocket centered at Γ and quasi 1D bands at the zone edges [1,2]. Extensive ARPES studies have shown that the CDW transition, setting in at 63 K [3], is mainly driven by the quasi 1D states, with the opening of a pseudo gap at the D point of the Brillouin zone. For this reason, Fermi Surface Nesting (FSN) between these states was proposed as the driving force of the transition. However, FSN alone does not properly explain the observed changes in the gap and in the 3D band with temperature [4]. We performed time and angle resolved photoemission spectroscopy (trARPES) measurements on ZrTe3 single crystals, probed with 6 eV and 20.9 eV photon energy, revealing a transient photoinduced energy shift of both the 3D and 1D states and subsequent coherent oscillation of the band structure compatible with the excitation of an Ag phonon mode. Hence, our experiment indicates the presence of a strong electron phonon coupling, that could be involved in the CDW formation, in agreement with complementary observations [5] and providing an alternative scenario to the nesting mechanism.

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