

Charge density waves in 2D materials

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Abstract

We explore via Density Functional Theory the electronic structure and the manifestation of charge density waves (CDWs) in 3 different single-layered transition metal dichalcogenides: TiSe_2 , NbSe_2 and TiTe_2 . Each of these materials presents a particularity from the viewpoint of behavioural spectra of 2D materials in the CDW phase. In the case of TiSe_2 is the stabilization of the structure from the combination of the phonon modes coming from three inequivalent M points. The effect of doping on TiSe_2 is dramatic and both electron and holes doping finally suppress the CDW phase. NbSe_2 shows a persistence of the CDW phase with doping unlike TiSe_2 and also a co-existence of different CDW phases. Finally TiTe_2 presents a strain-induced CDW phase stabilization.

References

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Figures

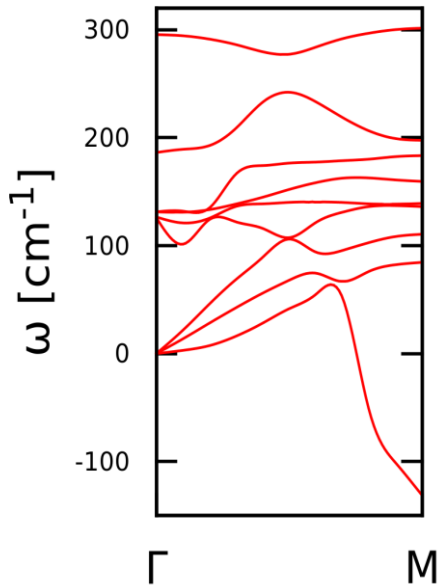


Figure 1: Phonon dispersion of the undistorted single-layered TiSe_2 in the Γ -M direction of the BZ.

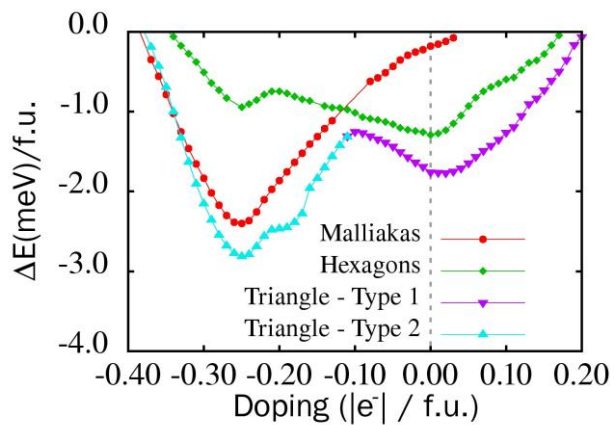


Figure 2: Charge-density wave phase ordering in single-layered NbSe_2 as a function of doping (negative values mean electron doping)