A first principles exploration of Charge Density Waves in 2D Transition Metal Dichalcogenides

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We explore by means of Density Functional Theory the electronic structure and the manifestation of Charge Density Wave (CDWs) in three different single-layered transition metal dichalcogenides: $TiSe_2$, $TiTe_2$ and $NbSe_2$. Each of these materials presents a particularity from the viewpoint of behavioral spectra of 2D materials in the CDW phase.

In the case of $TiSe_2$ we show that the prevailing stable phase of the CDW arises from the combination of the phonon modes coming from the three inequivalent M points[1]. The effect of charge doping on $TiSe_2$ single-layers indicates a suppression of the CDW phase for large enough values of both electrons, respectively doping.

$NbSe_2$ single-layers present an unexpected CDW phase where up to six different 3x3 modulations could be stabilized. From these six structures, three of them are experimentally found to coexist. In opposition with $TiSe_2$, $NbSe_2$ shows a persistence of the CDW phase with doping with both electrons and holes[3].

Finally, for the case of $TiTe_2$ we suggest that tensile bi-axial strain could stabilize the CDW phase starting from the single-layer configuration and going up to several layers[2].

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