Phonon Softening in the CDW Systems $NbSe_2$ and $TiSe_2$

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We investigated the soft-mode behaviour of phonons in the Charge Density Wave (CDW) systems $NbSe_2$ and $TiSe_2$ both theoretically in Density Functional Theory (DFT) based on ab-initio phonon calculations and experimentally by means of high resolution Inelastic X-ray Scattering (IXS). For both materials, the theoretical predictions for the phonon softening using the experimental lattice parameters coincide with the experimentally observed CDW instability behaviour. While $TiSe_2$ shows a rather sharp phonon anomaly at T = 190 K, the anomaly in $NbSe_2$ at T = 33 K is much broader than expected for a Fermi surface nesting driven CDW instability. For $NbSe_2$, we exclude Fermi surface nesting as main origin of the phonon softening. For $TiSe_2$, there is no need to go beyond DFT in order to describe the phonon softening.