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Charge-Density Wave and Superconducting Dome in $TiSe_2$ from Electron- Phonon Interaction MATTEO CALANDRA, MAURI FRANCESCO, CNRS and Université P. et M. Curie — At low temperature TiSe2 undergoes a charge-density wave instability. Superconductivity is stabilized either by pressure or by Cu intercalation. We show [1] that the pressure phase diagram of TiSe2 is well described byfirst-principles calculations. At pressures smaller than 4 GPa charge-density wave ordering occurs, in agreement with experiments. At larger pressures the disappearing of the charge-density wave is due to a stiffening of the short-range force constants and not to the variation of nesting with pressure. This suggests a common origin of the charge density waves instability in transition metal dichalcogenides, as also demonstrated in previous works by first principles calculations on bulk and few layers NbSe2 [2]. In TiSe2, the behavior of Tc as a function of pressure is entirely determined by the electron-phonon interaction without need of invoking excitonic mechanisms. Our work demonstrates that phase diagrams with competing orders and a superconducting dome are also obtained in the framework of the electron-phonon interaction.
[1] M. Calandra and F. Mauri, PRL 106, 196406 (2011)
[2] M. Calandra, I. I. Mazin and F. Mauri, PRB 80, 241108(R) (2009)

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