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Charge Density Waves in the bulk and mono-layer VSe₂ YANG-HAO CHAN, CHING-MING WEI, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan, MEI-YIN CHOU, School of Physics, Georgia Institute of Technology, USA — Charge density waves (CDWs) are widely observed in the layered transition-metal dichalcogenides (TMDs). With the capability of preparing atomically thin samples in the experiment, the underlying mechanism of the formation of CDWs and the role played by dimensionality in TMDs can now be studied in great detail. We present the first-principles calculations on bulk and mono-layer VSe₂. Our results agree with the experimental findings that the dominant CDW phase has a 4x4x3 supercell structure in the bulk system. Electronic structure calculations suggest Fermi-surface nesting is a relevant mechanism. On the other hand, we find a new $3\sqrt{3}\times\sqrt{3}$ CDW phase as the lowest energy structure in the mono-layer case induced by strong electron-phonon interaction. We also find that substantial hole doping leads to a CDW-superconducting (SC) phase transition. The SC transition temperature is predicted to be higher than that of the bulk from our first-principles calculations.

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