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The effect of dimensionality on the charge-density-wave phase in layered dichalcogenides[1] DARSHANA WICKRAMARATNE, PRADYUMNA GOLI, ALEXANDER BALANDIN, ROGER LAKE, University of California, Riverside — Transition-metal dichalcogenides exhibit a variety of conducting phases, which includes a charge-density wave state (CDW). Exfoliation of these layered materials allows the effect of dimensionality on the CDW state to be studied. CDW collective states are currently being considered as an alternative state variable for information processing [1]. 2H-$TaSe_2$ and 1T-$TiSe_2$ are examples of layered transition metal dichalcogenides that undergo a CDW transition. Our recent experiments demonstrated an increase in the CDW transition temperature of $TiSe_2$ with a decrease in film thickness [1]. This increase in temperature was attributed to the negative coefficient of the CDW transition temperature-pressure relationship. Here we present a density-functional theory investigation of the CDW instability in bulk, single and few-layer 1T-$TiSe_2$ and other layered dichalcogenide materials. The effect of the film thickness on the atomic structure, electronic structure, electron-phonon coupling and the CDW transition temperature will be discussed for each material.

[1] Goli, P., Khan, J., Wickramaratne, D., Lake, R. K., & Balandin, A. A. (2012). Charge Density Waves in Exfoliated Films of Van der Waals Materials: Evolution of Raman Spectrum in $TiSe_2$. Nano Letters.

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