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First-principles Studies of Multiple CDW Phase in 1T-$TaTe_2$ Monolayer

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The spontaneous formation of electronic orders is a crucial element for understanding complex quantum states and engineering heterostructures in 2D materials. The enhanced electron-electron and electron-phonon interactions due to quantum confinement and reduced screening in 2D materials often result in complex electronic phases distinct from the corresponding bulk systems. Among TMDCs, TaX_2 (X=S, Se) has been extensively studied as a prototypical material to explore the role of strong electron correlation in an electron-phonon coupling driven CDW system. Despite being in the same family of Ta-based dichalcogenides, 1T-$TaTe_2$ has been relatively less investigated. In this material, the stronger Te-Te interlayer coupling would likely create distinct electronic and structural features compared to those of TaS_2 and $TaSe_2$. In this study, we investigated the type of CDW phase that may emerge when the strong Te-Te interlayer coupling gets completely removed in ML 1T-$TaTe_2$. Here, our density functional theory calculation reveals that ML 1T-$TaTe_2$ show a variety of metastable CDW phases, including 3×3, √13×√13, and √19×√19 superstructures. The phonon spectra and electron susceptibilities will be discussed and associated underlying mechanism will be introduced in detail.

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