Lattice Instability and Charge Density Wave Phases of Monolayer 1T-VSe_2

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Transition-metal dichalcogenides (TMDCs) have attracted researchers due to their peculiar phenomena, including superconductivity, metal-insulator transition, and charge density wave (CDW) order [1-4]. TMDCs comprise transition-metal atoms (M: Mo, W, V, *etc*) and group-VI chalcogen atoms (X: S, Se, and Te) with the formula unit of MX_2. Monolayer (ML) 1T-VSe_2 has been extensively investigated due to recent observations of varying CDW order compared with bulk. Bulk 1T-VSe_2 has been known to show the $4\times4\times3$ CDW order with a transition temperature (T_c) of 110K [4, 5]. Differently from bulk, the ML 1T-VSe_2 was reported to show a CDW phase of $\sqrt{7}\times\sqrt{3}$ periodicity with increased T_c, whose possibility was supported theoretically [6, 7]. Also reported is the emergence of a CDW phase comprising alternating $2\times\sqrt{3}$ and $\sqrt{7}\times\sqrt{3}$ superstructures with a full gap in ML 1T-VSe2 [8, 9]. The atomic structure of these CDW phases and the mechanism of CDW transition are still veiled. This work will present the results of first-principles calculations on the ML 1T-VSe2. The calculated phonon dispersion relation reveals the existence of a few unstable modes. We will address the formation of CDW phases, which are period-increasing structural modifications, due to unstable phonon modes, the energetic stability of investigated CDW phases, and the electronic structure of CDW phases. Finally, we will compare the simulated scanning tunneling microscope (STM) images with the available experimental STM images.

References

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