Discovery of 2D Mott insulating phase in 1*T*-$NbSe_2$ atomic layer

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Layered transition-metal dichalcogenides (TMDs) have been a target of intensive studies for more than half century since they exhibit a variety of physical properties depending on the combination of elements or the crystal structure such as 1*T* and 2*H* phases [1]. Recent efforts to fabricate atomic-layer counterpart of TMDs gave rise to exotic physical properties distinct from bulk. Among the TMDs, 2*H*-$NbSe_2$ has attracted much attention since it simultaneously exhibits charge density wave (CDW) and superconductivity [2]. In contrast, 1*T*-$NbSe_2$ has not been studied yet because of the difficulty in synthesizing the unstable 1*T* phase [3,4].

Here we report an angle-resolved photoemission spectroscopy (ARPES) study of monolayer $NbSe_2$ epitaxially grown on bilayer graphene. We have succeeded for the first time in selectively fabricating monolayer 2*H*- and 1*T*-$NbSe_2$, and clarified the electronic structure by ARPES [5]. Figure 1 shows the valence-band ARPES intensity plots along the Γ-M cut for monolayer (a) 2*H*- and (b) 1*T*-$NbSe_2$. We found that monolayer 2*H*-$NbSe_2$ exhibits metallic behavior, while 1*T*-$NbSe_2$ shows insulating behavior in sharp contrast to the band theory which predicts the metallic state with half-filled bands. In order to clarify the origin of such unconventional electronic states, we have performed scanning tunneling microscopy (STM). Figure 2 displays constant current STM images of monolayer (a) 1*T*- and (b) 2*H*-$NbSe_2$. We have found that monolayer 1*T*-$NbSe_2$ exhibits CDW with $\sqrt{13}\times\sqrt{13}$ periodicity, distinct from 3x3 CDW in 2*H* counterpart.

In the presentation, we will show detailed ARPES and STM results, and discuss the origin of novel insulating state in 1*T*-$NbSe_2$ in terms of 2D Mott insulating state.

References

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Figures

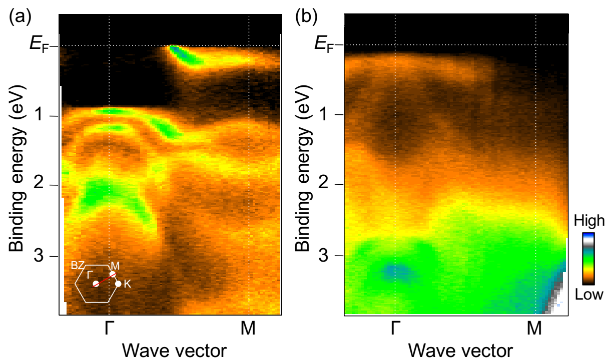

Figure 1. ARPES-intensity plots along the Γ-M direction as a function of wave vector and binding energy for monolayer (a) 2*H*- and (b) 1*T*-$NbSe_2$ at 40 K.

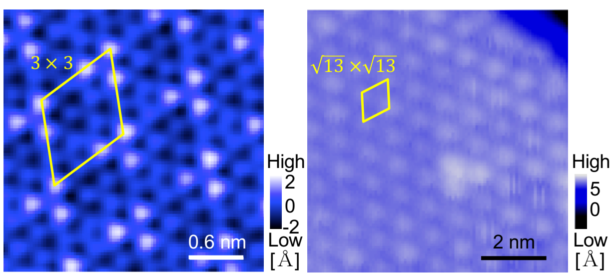

Figure 2. Constant current STM images of monolayer (a) 2*H*- and (b) 1*T*-$NbSe_2$ at 4 K.