Chapter 5
Conclusions and Prospect

Abstract As a summary of contents, the major research results and outlooks are included in this chapter.

Keywords Germanene · Hafnium honeycomb · $PtSe_2$ · 2D materials

Graphene was most highly studied in material-related science in the past dozen years because of its exceptional properties and wide applications. More importantly, the rise of graphene initiated a new field—two dimensional (2D) materials. The explosive studies on graphene have inspired considerable interests towards graphene-analogous 2D materials. It is in this background that this thesis aims at investigating novel 2D atomic crystals beyond graphene. A variety of surface-science techniques including LEED, STM, STEM, XPS, ARPES, and Raman spectroscopy combined with DFT calculations are employed to systematically study three new graphene-like 2D materials—germanene, hafnene, and $PtSe_2$. The major research results and outlooks are summarized as follows.

(1) The experimental synthesis of germanene, a germanium-based counterpart of graphene, is reported for the first time, which is the third single-element 2D material following graphene and silicene. A ($\sqrt{19} \times \sqrt{19}$) superstructure with respect to the Pt(111) substrate is observed by LEED and STM, which coincides with the (3 × 3) superlattice of a buckled germanene sheet demonstrated by the first-principle calculations. The calculated electron localization function reveals that adjacent Ge atoms directly bind to each other, confirming the continuity of 2D germanene sheets on the Pt(111) surface. This work develops the first method of preparing single-layer germanene and facilitates the subsequent experimental studies on its physical properties and potential applications.
(2) The first honeycomb structure composed of transition metals-hafnene-is experimentally fabricated on an Ir(111) surface using UHV-MBE method. Theoretical calculations reveal interesting ferromagnetism, high density of d states at the Fermi level, and large spin-splitting of the Dirac cones for a freestanding Hf honeycomb structure, indicating rich electronic, magnetic and catalytic potential

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applications. The realization and investigation of hafnene broaden the scope of artificially synthesized honeycomb structures and offer a new platform for studying hitherto unknown quantum phenomena and electronic behaviors in 2D systems.

(3) Single-layer $PtSe_2$ films, a new transition metal dichalcogenide (TMD) crystal, are prepared through direct selenization of a Pt(111) substrate. Multiple experimental characterizations and DFT calculations depict the structural and electronic properties of monolayer $PtSe_2$. The high photocatalytic activities measured experimentally make $PtSe_2$ single layers promising materials in optoelectronics and photocatalysis. Moreover, monolayer $PtSe_2$ exhibits circular polarization in momentum space, indicating potential applications for valleytronic devices. These studies are a significant step forward in enriching the family of single-layer semiconducting TMDs and exploring their application potentials in photoelectronic and energy-harvesting devices.