Tuneable Electronic Structure of Atomically Resolved Two-Dimensional III-VI Alloys

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Abstract

Doping and alloying is a powerful method to tune the chemical and physical properties of two-dimensional (2D) semiconductors[1–4]. In order to correlate structure-property relationship of 2D multispecies alloys, it is the key to Visualize their atomic structure. However, revealing the atomic registry of an alloy becomes more challenging as the number of atomic planes and atomic species increase. Here, we uncover the atomic-scale crystal structure and stacking sequence of monolayer and few-layer III-VI alloys using annular dark-field scanning transmission electron microscopy (ADF-STEM) imaging combined with image simulation, second harmonic generation (SHG), and first principles calculations. Using low-loss electron energy loss spectroscopy (EELS) and density functional theory (DFT) calculations, the atomic and electronic structure of $GaSe_{0.5}Te_{0.5}$ alloys with different layer numbers will be correlated. The electronic bandgap is found, experimentally and theoretically, to be sensitive to layer number. Moreover, the energy of the π plasmon peak and the intensity of the π + σ plasmon peak are determined to be significantly affected by the number of layers.

References

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Figures

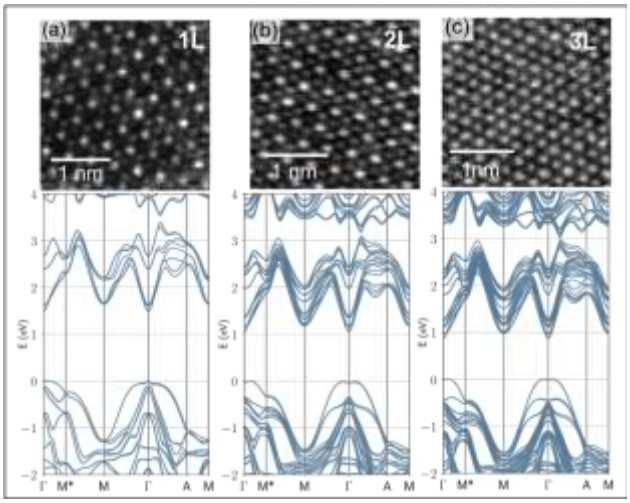

Figure 1: Atomic-resolution ADF-STEM images of (a) monolayer, (b) bilayer, and (c) trilayer $GaSe_{0.5}Te_{0.5}$ crystals and their corresponding calculated DFT-PBE Kohn-Sham band structures.