Supplementary information:

A 2D bismuth-induced honeycomb surface structure on GaAs(111), by Yi Liu et al.

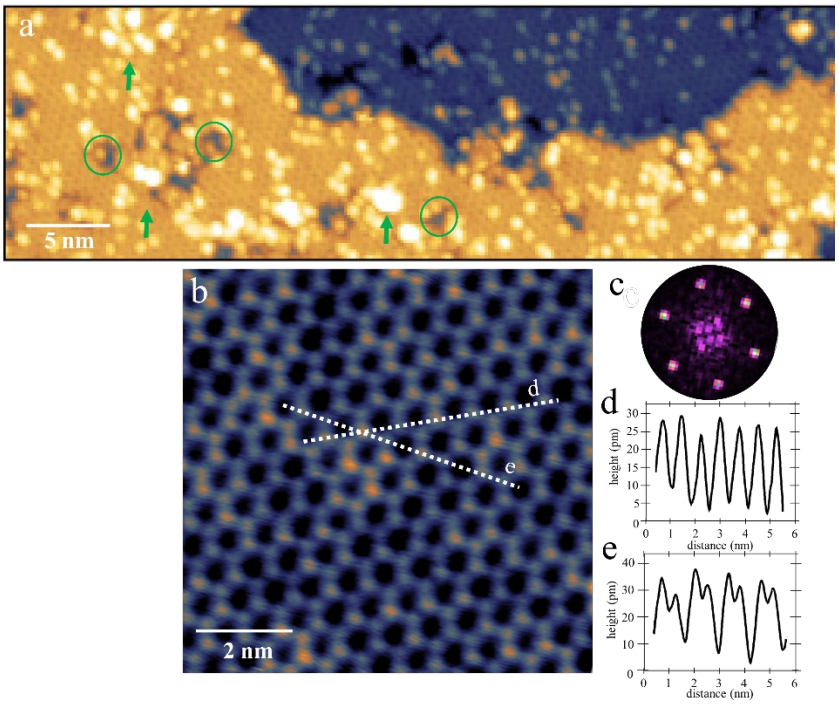

Figure 1: Honeycomb structure upon Bi deposition on GaAs(111)B at 250°C (a) Overview STM image and (b) atomically-resolved STM image of the honeycomb structure. Green circles (arrows) in (a) indicate some hollow areas (Bi clusters) on the surface. Each bright dot in (b) presents an individual Bi atom. (c) Fast Fourier transform (FFT) image of image (b), showing a clear single periodicity of 6-folded symmetry. (d) and (e) Height profiles of line scans across the honeycomb structure as indicated in (b) by white lines. STM color scale extends over 44 pm in (b). V_T= -3V, I_T= 50 pA for (a) and V_T= -5 V, I_T= 100 pA for (b).

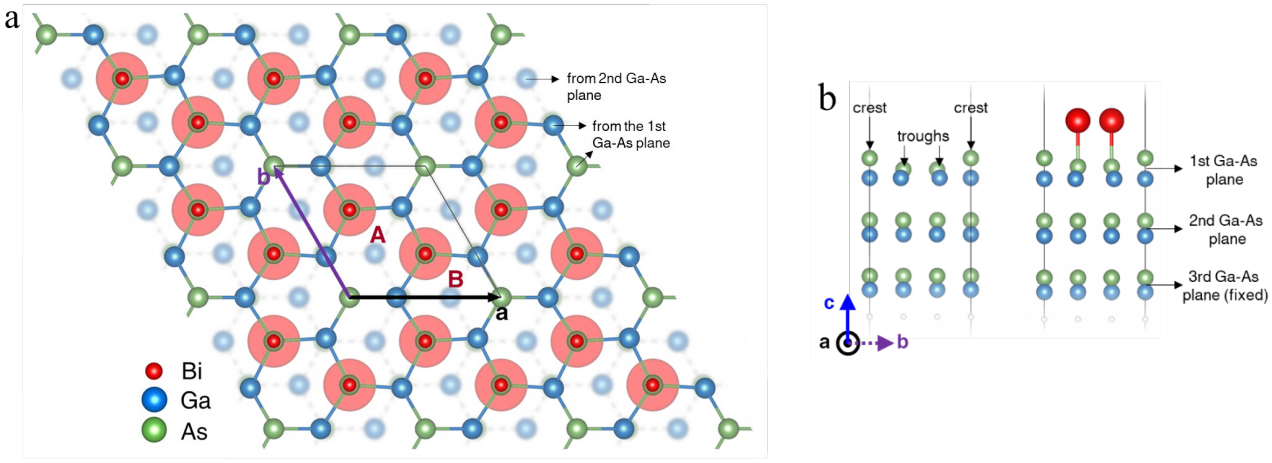

Figure 2: **First-principles atomistic model of the Bi honeycomb structure.** (a) shows the top view of the Bi-induced honeycomb structure on top of the GaAs(111)B substrate. The positions of the Bi atoms are emphasized with shaded red circles to highlight its honeycomb lattice that is made up of two sublattices, A and B. The hollow site is set as the origin of the unit cell of the honeycomb lattice structure and **a** and **b** define the lattice vectors of the unit cell. (b) shows the side view of the GaAs(111)B substrate with (right) and without (left) the honeycomb lattice. The first two Ga-As planes of the substrates are fully relaxed by minimizing the total energy of the system while the third plane is fixed in position to model the bulk