# Large-area single-crystals of borophene on square and triangular Copper surfaces: synthesis and characterization

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The materials-by-design paradigm is based on synergistic efforts involving synthesis, characterization and advanced computation to ensure materials meet technological needs within a cost-effective framework. Borophene, a crystalline monolayer sheet, is envisaged to play an important role in this area because of its extraordinarily rich polymorphism. The multitude of potentially stable structures singles out borophene from all other two-dimensional materials and fuels hopes for obtaining on-demand structures with applications in flexible electronics, energy storage or catalysis.

We have used a unique ultra-high vacuum system for synthesis, by Molecular Beam Epitaxy, and in-situ characterization, by Low Energy Electron Microscopy, of micron-size borophene crystals on Cu(111) and Cu(100) substrates. Our real-time imaging capabilities provide information about the growth of faceted borophene islands up full monolayer coverage and also about phase-stability, evaporation and sub-surface dissolution. Combining low energy electron diffraction with scanning tunneling microscopy and ab initio theory allows us to resolve the crystal structures as triangular networks with vacancy ratios $\eta$ = 1/5 for Cu(111) and $\eta$ = 1/6 for Cu(100) surfaces. First-principles calculations indicate that charge transfer rather than covalent bonding, couples borophene to the underling Cu surfaces. The calculated electronic band structures host multiple anisotropic Dirac cones. Ex-situ scanning near-field optical microscopy data reveal dielectric contrast between borophene and substrates, showing that nano-optical tools provide new ways to access intrinsic electronic properties of these novel structures.

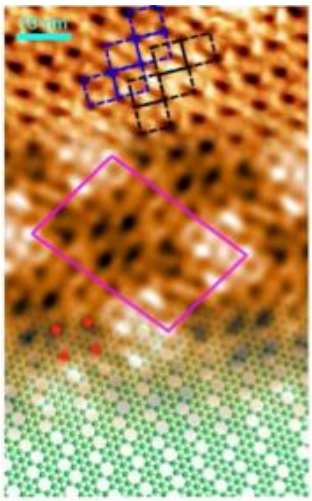

Figure: Continuous transition from experimental STM topography to the simulated STM image to the atomic model for B/Cu(100)

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