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# Boron nitride on Cu(111): an electronically corrugated monolayer

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Abstract: Ultrathin films of boron nitride (BN) have recently attracted considerable interest given their successful incorporation in graphene nanodevices and their use as spacer layers. to electronically decouple and order functional adsorbates. Here, we introduce a BN monolayer grown by chemical Vapor deposition of borazine on a single crystal Cu support, representing a model system for an electronically patterned but topographically smooth substrate. Scanning tunneling microscopy and spectroscopy experiments evidence a weak bonding Of the single BN sheet to Cu, preserving the insulating character of bulk hexagonal boron nitride combined with a periodic lateral variation of the local work function and the surface potential. Complementary, density functional theory calculations reveal a varying registry of the BN relative to the Cu lattice as origin of this electronic Moire-like superstructure.

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# Supporting Information

# Boron nitride on Cu(111): An electronically corrugated monolayer

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## Experimental procedures and theoretical methods

All experiments were performed in a custom-designed ultrahigh vacuum (UHV) apparatus comprising a commercial low-temperature CreaTec STM [1] based on a design described in ref. [2]. The system base pressure is below $2 \times 10^{-10}$ mbar. The Cu(111) single crystal surface was cleaned by repeated cycles of $Ar^+$ sputtering (800 eV) followed by annealing to 1000 K. Subsequently, BN (sub)monolayers were prepared by decomposition of borazine $(HBNH)_3$ on the hot Cu(111) surface, following a recipe described in detail in previous publications [3, 4]. Importantly, the BN growth is self-saturating when a complete monolayer coverage is reached. During borazine dosage, the Cu(111) crystal was kept at temperatures between 983 K and 1120 K. Generally, the higher temperatures favor larger BN domain sizes and thus reduce the defect density, but go in hand with desorption of Cu from the crystal surface. For full BN layers, the sample was typically exposed to ~800 L of borazine. For sub-monolayer coverages, exposures down to 40 L were applied. After the borazine dosage, the sample was cooled down and transferred into the STM, where constant current images were recorded at T ~ 6 K using electrochemically etched tungsten tips. In the figure captions $V_b$ refers to the bias voltage applied to the sample and $I$ to the tunneling current. Differential conductance

data (dI/dV spectra and maps) were obtained by lock-in technique with a bias modulation amplitude of 18 mV rms and a frequency of 969 Hz (spectra) and 2.97 kHz (maps). To cover the large voltage range mandatory to measure high-order field emission resonances, the feedback loop was kept closed for the dI/dV point spectroscopy. The fast fourier transformation (FFT) uses the WSxM software. [5]

Density Functional Theory (DFT) calculations were carried out within the Gaussian-Plane Waves (GPW) formalism[6] as implemented in the CP2K package [7]. The revised PBE functional [8] was used to treat the exchange-correlation energy in combination with the Grimme D3 correction [9] to account for dispersive interactions. Double-Zeta valence polarized basis sets of the MOLOPT [10] type were used for all elements, together with Goedecker-Teter-Hutter pseudopotentials [11]. 11, 3, and 5 electrons were considered explicitly in the valence for Cu, B, and N, respectively. The energy cut-off of the plane wave expansion of the density was set to 500 Ry, and a 20 Å vacuum region was used for surface models in a slab geometry. Commensurate adsorption on Cu was studied using 7-layer Cu(111) slabs with a monolayer of BN on both sides; because the Brillouin zone is only sampled at the Γ-point, the simulations contain laterally a 6x6 supercell.

## Projected Density of States

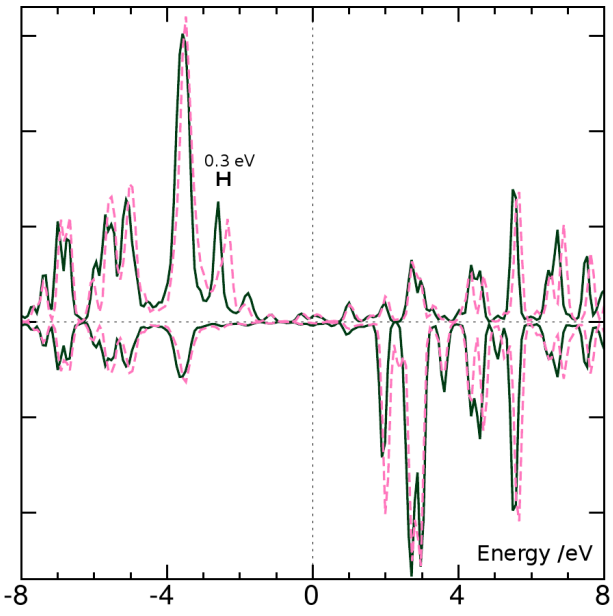


Figure S1. Projected Density of States (PDOS) of $p_z$ orbitals on nitrogen (positive y axis) and boron (negative y axis) for BN in $B_{fcc}N_{top}$ (continuous line) and $B_{fcc}N_{hcp}$ (dashed line) registries. The 0.3eV shift of the highest occupied molecular orbital (HOMO) peak is highlighted.

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