

Graphene on Rh(111): combined DFT, STM and NC-AFM studies

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Graphene, a single layer of carbon atoms ordered in a "chicken-wire" lattice [1], is proposed to be used in many technological applications. Among them are gas sensors, THz-transistors, integrated circuits, touch screens, and many others. One of the promising systems on the basis of graphene is its interface with metallic substrates [2]. Here graphene can be used as a protection layer for the underlying substrate, as a spin-filtering material separating two layers of a ferromagnetic material, or, in case of its growth on a lattice mismatched surfaces [for example, Ir(111), Rh(111), or Ru(0001)], as a template for the preparation of ordered arrays of clusters. For graphene on Rh(111) [Fig.1(a-c)] several regions of different arrangements of carbon atoms above a Rh(111) substrate can be found: ATOP [A; carbon atoms are above Rh(S-1) and Rh(S-2) atoms], HCP [H; carbon atoms are above Rh(S) and Rh(S-2) atoms], FCC [F; carbon atoms are above Rh(S) and Rh(S-1) atoms], and BRIDGE [B; Rh(S) atoms bridge the carbon atoms]. These places are marked in Fig.1(a) by circle, down-triangle, square, and stars, respectively. Among them, the BRIDGE positions are expected to be the most energetically favorable for the nucleation of deposited atoms on top of a graphene layer. The nowadays available force spectroscopy and microscopy can shed light on this problem and can be used as a tool, which helps to optimize the preparation of ordered arrays of clusters on a graphene template. In this contribution we present the combined study of the graphene/Rh(111) system via application of the state-of-the-art DFT calculations, STM, and NC-AFM. The calculated imaging contrast for STM between all high-symmetry positions for graphene/Rh(111) is in very good agreement with experimental results and this contrast does not depend on the sign of the bias voltage applied between a tip and the sample. As opposed to the latter observation, the imaging contrast in atomically-resolved AFM measurements depends on the frequency shift of the oscillating tip that can be understood on the basis of measured force-spectroscopy curves. The presented results are compared with the available theoretical data.

References

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