EDGE EFFECTS IN GRAPHENE NANOISLANDS ON Co(0001) PROPED BY STM MEASUREMENTS AND FIRST PRINCIPLES CALCULATIONS

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We recently demonstrated the growth of regularly shaped, nanoscale islands of graphene on Co(0001) surfaces [Fig. 1(a) and Ref. 1]. Here we combine low-temperature scanning tunneling microscopy (STM) measurements and DFT based calculations to study their edge properties [2]. These nanoislands reveal a well-ordered structure with predominant zigzag termination at the edges, as opposite to what is predicted to be the most stable configuration in isolated systems [3]. Moreover, STS tunneling spectra show prominent peaks at low bias, where the edges dominate the images. DFT calculations provide insights into the relative stability of different edge configurations and passivation conditions [Fig. 1(b-e)], as driven by interactions with Co. The coupling with the substrate results also in a dramatic modification of both electronic and magnetic properties at the edges. In particular, the edge-localized spin polarization typical of isolated zigzag edges [4] is strongly suppressed by the interaction with the magnetic substrate. In order to study hybridization and size effects, we transform to localized Wannier states and develop a minimal model for the effective π states of these graphene nanostructures [5].

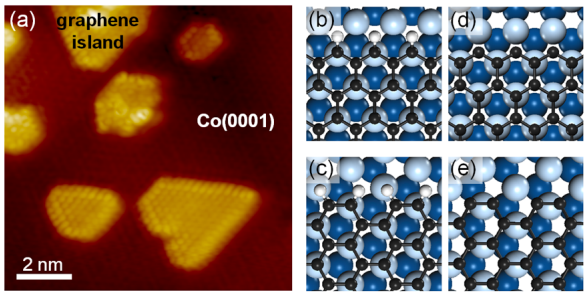

Figure 1: (a) Typical STM image of graphene flakes grown on a Co(0001) surface. The image was taken at 4.9 K with a sample bias of -6 mV. (b-e) Schematic of zigzag (b,d) and armchair (c,e) edges of graphene flakes on Co(0001), with (b-c) and without (d-e) hydrogen passivation, after relaxation through DFT total energy methods. Carbon atoms are in dark grey; the topmost and the second layer cobalt atoms are in light and dark blue, respectively; H is in white.

References

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