Edge effects in graphene nanoislands on Co(0001) probed 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 [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, 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 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.

References

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