Structure of Epitaxial graphene Moiré coincidence network; lattice mismatch versus surface strain

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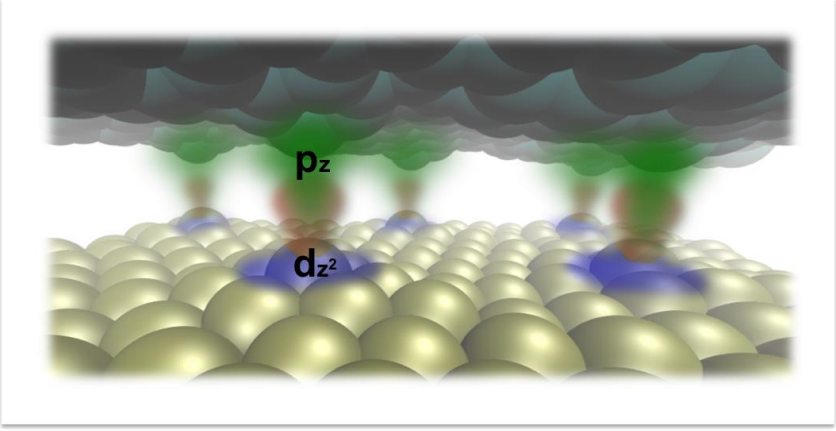
Epitaxial graphene can be efficiently grown on transition metal surfaces leading to the formation of coincidence superstructures (Moirés) exhibiting different sizes and orientations with respect to the substrate. In this work we aim to understand the modification of the graphene atomic and electronic properties induced by the interaction with the underlying surface. Firstly, we will address the problem of how many Moirés superstructures can be accommodated on a particular metal surface. To this goal, we have grown submonolayer coverage of multi-domain epitaxial graphene islands on Pt(111) by low-temperature decomposition of large organic precursors [1] and observed them by STM. We present a purely simple geometric model that predicts that graphene can only grow at those angles at which the mismatch between the graphene and the metal networks is minimized [2]. This model was developed for the case of Pt(111), and successfully applied to other metals and found to work with most substrates[3]. However, there are several aspects that remain unclear, as why the mismatch, and not the strain, is ruling the stability of these structures. We have performed full DFT calculations that lead us to the conclusion that for all reported Moirés the system relaxes inducing a non-negligible atomic corrugation both, at the graphene and at the outermost platinum layer [4].



Formation of an anti-Moiré network of pinning points.

[1] Otero et al., Phys Rev. Lett. 105, 216102 (2010)
[2] Merino et al., ACS Nano 5, 5627-5634 (2011)
[3] Merino et al., ACS Nano 8, 3590-3596 (2014)
[4] Martinez et al. submitted