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Graphene's striped moire acting as a switchman for metal adatoms

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Graphene (G) grown on Ni(100) forms the stripped moiré pattern that can be described as an alternate arrangement of valleys, where G is close to the nickel substrate and interacts with it rather strongly, and ridges, where G is far away from the substrate and is almost free-standing [1]. When metal adatoms are deposited on G/Ni(100), the structural differences between the valleys and the ridges reflect in the adsorbate's behavior as well. The scanning-tunneling microscopy (STM) measurements of cobalt (Co) deposited on G/Ni(100) revealed an abundance of Co on ridges and almost no Co on valleys. With the additional manipulation by the STM tip, Co clusters on ridges were able to move but only in a direction parallel to the stripes. Puzzled by this strong preference for ridges, we employed density functional theory (DFT) to model the different Co structures on G/Ni(100) [2]. From the DFT charge analysis we found that Co upon adsorption donates electrons to G and becomes positively charged both on valleys and ridges. Given that nickel substrate donates electrons to G as well, the charge redistribution in the system results in the Co-Ni repulsion modulated by G's corrugation - the farther is the Co adatom from Ni the weaker is the repulsion and thus the higher is the binding energy of Co on G. Moreover, the same repulsion increases the Co mobility, as the calculated barrier for the Co diffusion along the ridge is the lowest of all possible directions on the G's surface. This explains why the Co adatoms and small clusters remain on the ridge even after being kicked by STM tip. On the other hand, gold (Au) adatoms display the opposite behavior as they adsorb on G's valleys. Again here, the adsorbate-substrate electrostatic interaction explains the preference for valleys: unlike Co, Au adatoms take the electrons from G, resulting in the Au-Ni attraction that drives Au adatoms to the valleys as regions that are closest to the substrate. This leads us to the simple law: metal adatoms that donate electrons to G will adsorb on ridges whereas those that take electrons from G will adsorb on valleys, revealing the switchman's role of G's striped moiré for the positively/negatively charged adsorbates. This law is quite general as our DFT calculations show that it holds for many different elements from the periodic table. Our findings expand the possibilities in efforts for creating the self-assembled and well-ordered superlattices of metallic nanostructures using moiré graphene as template [3,4], as they reveal the preferred clusterisation sites and directions of diffusion for different types of atoms on stripe moiré graphene.

References

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Primary author: STAVRIĆ, Srdjan (CNR-SPIN)

Co-authors: Mr DEL PUPPO, Simone (University of Trieste); Mr CHESNYAK, Valeria (University of Trieste / CNR-IOM); Dr PANIGHEL, Mirco (CNR-IOM); Dr AFRICH, Cristina (CNR-IOM); Prof. PERESSI, Maria (University of Trieste)

Presenter: STAVRIĆ, Srdjan (CNR-SPIN)

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