Ni_2C formation at the graphene/Ni(111) interface: a first-principles investigation

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The peculiar graphene properties are very sensitive to its coupling with the substrate. In case of graphene (Gr) grown on Ni(111) surface, this is strongly affected by the formation of an intercalated carbide (Ni_2C) layer, which, remarkably, occurs only under rotated graphene (RG) and not under epitaxial graphene (EG) domains [1,2]. We performed first principles simulations based on density functional theory to explain the preferential surface segregation of the Ni-dissolved C atoms under rotated graphene domains [3]. Furthermore, a complete description of the electronic properties of Gr with and without carbide, in rotated and epitaxial domains is obtained. The atomic projected density of states confirms that carbide formation decouples Gr from the substrate and restores its semi-metallic nature. Finally, we obtained the specific C1s core level shifts that are the fingerprints of different Gr/Ni_2C/Ni(111) configurations in good agreement with the experimental results.

This research is partially funded by a grant from the Italian Ministry of Foreign Affairs and International Cooperation (Project of Particular Relevance, Italy – Republic of Serbia).

REFERENCES

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FIGURES

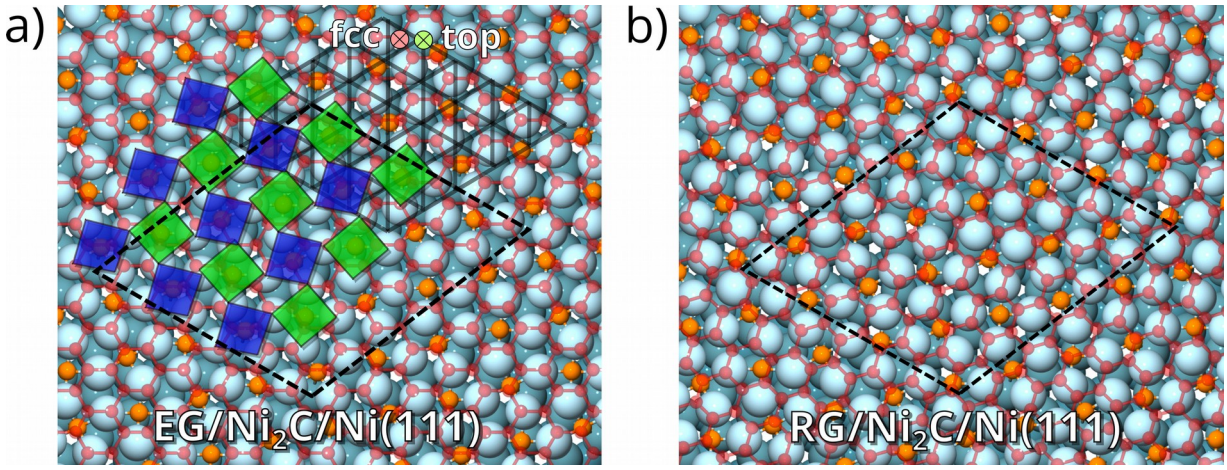

Figure 1: The structure of Ni_2C at Ni(111) under epitaxial graphene (EG, left panel) and rotated graphene (RG, right panel). C atoms of graphene are represented by small transparent red spheres and C atoms of carbide as larger orange spheres. Ni atoms of carbide are represented by big light blue spheres, and Ni atoms of Ni(111) by blue spheres. The “clock reconstruction” of carbide is emphasized with green and dark blue squares. The Ni(111) lattice, not clearly visible under carbide, is denoted by black network in the upper part of the left panel. The unit cell depicted with dashed black lines has been carefully identified to accommodate the three different lattices (Ni(111) substrate, carbide layer, graphene overlayer) both in case of epitaxial and rotated graphene.