JULY 07, 2020
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Graphene Online &2DM Fundamental Research Insights
GO 2020

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

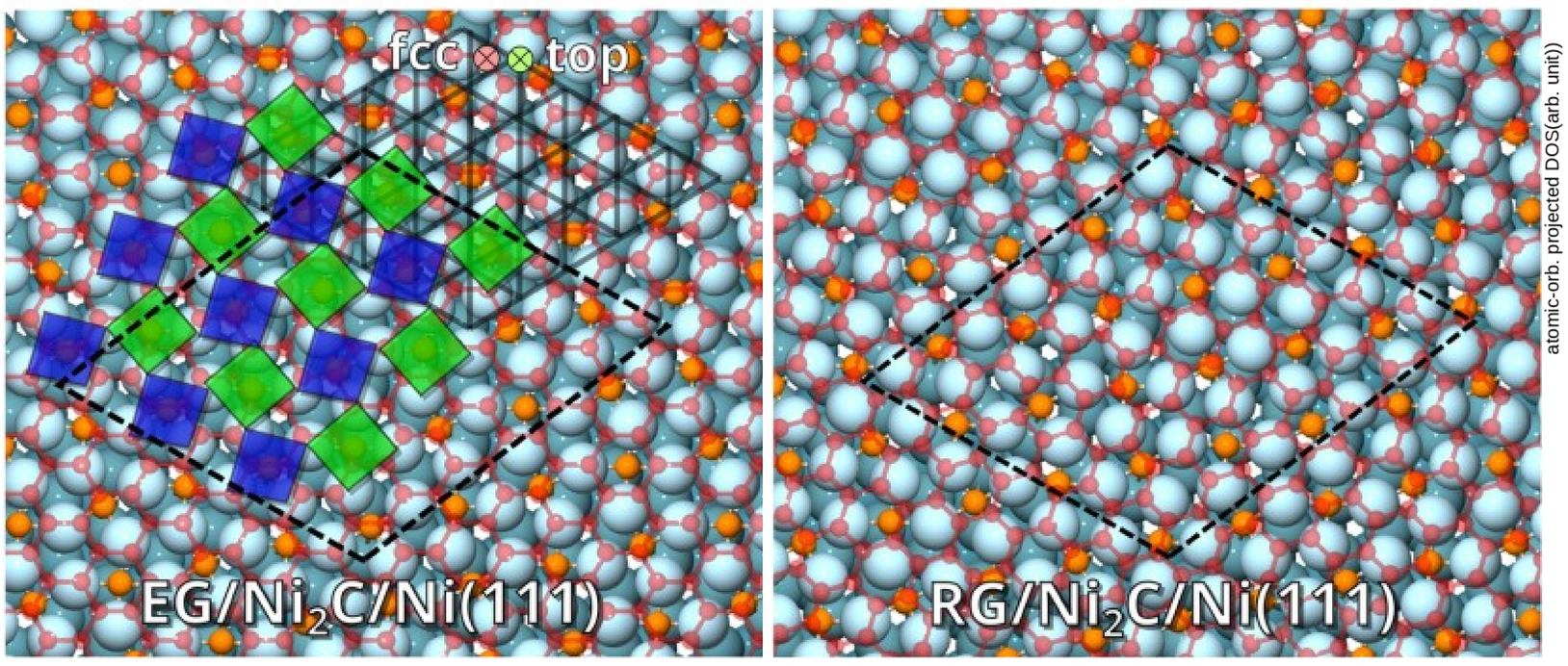
Simone Del Puppo[1],Srdjan Stavrić [1,2],Željko Šljivančanin [2], Maria Peressi [1]

[1]Department of Physics, University of Trieste, via Valerio 2, I-34127 Trieste, Italy
[2]Vinča Institute of Nuclear Sciences, University of Belgrade, P. O. Box 522, RS-11001, Republic of Serbia

ABSTRACT

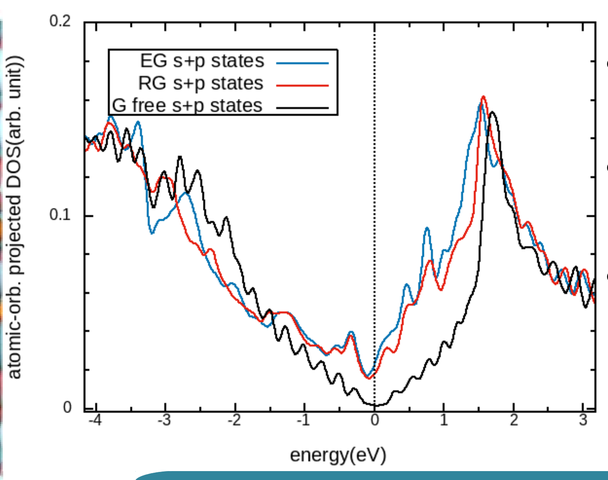
The peculiar graphene(G) properties are very sensitive to its coupling with the substrate. In case of G grown on Ni(111) surface, this is strongly affected by the formation of an intercalated carbide (Ni_2C) layer, which, remarkably, occurs only under rotated graphene (RG) and not under epitaxial graphene (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 RG domains [3]. Furthermore, a complete description of the electronic properties of G with and without carbide, in RG and EG domains is obtained. Finally, we obtained the specific C1s core level shifts that are the fingerprints of different G/Ni_2C/Ni(111) configurations in good agreement with the experimental results.

STRUCTURE



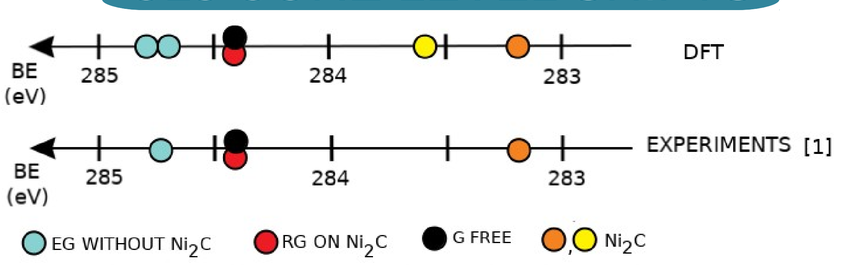
- simulation cell: 6 x(√43 R 7°.6)
- matching three different lattices (and G with two different orientations)
- Ni_2C is stable under both EG and RG
- Ni_2C detaches both EG and RG from Ni

ELECTRONIC PROPERTIES



- Dirac Cones preserved
- G nearly free-standing
- E_F shift: 0.1 eV

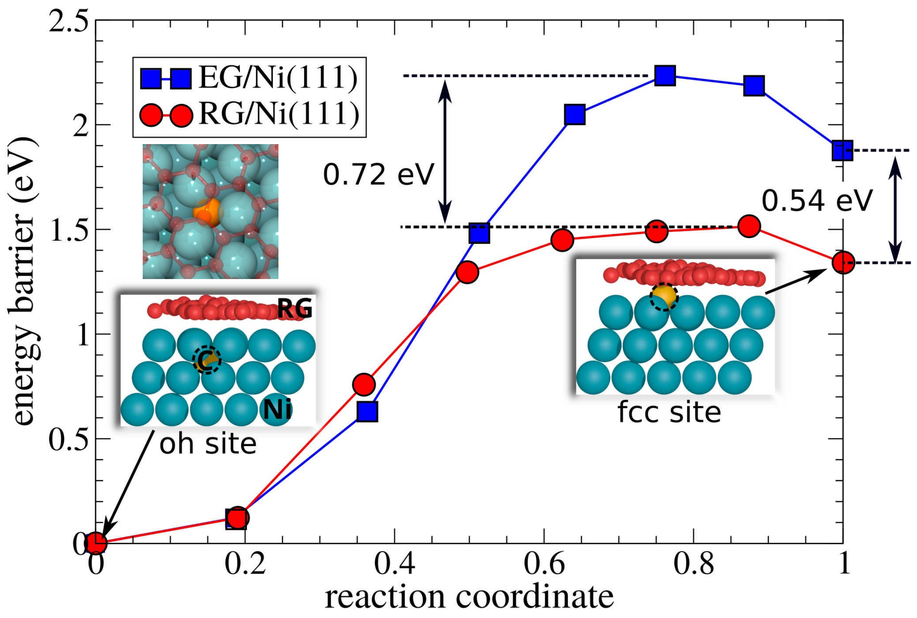
C1s CORE LEVEL SHIFTS



- fingerprint of different chemical environment
- two different CLS for carbide are found
- agreement th./exp.

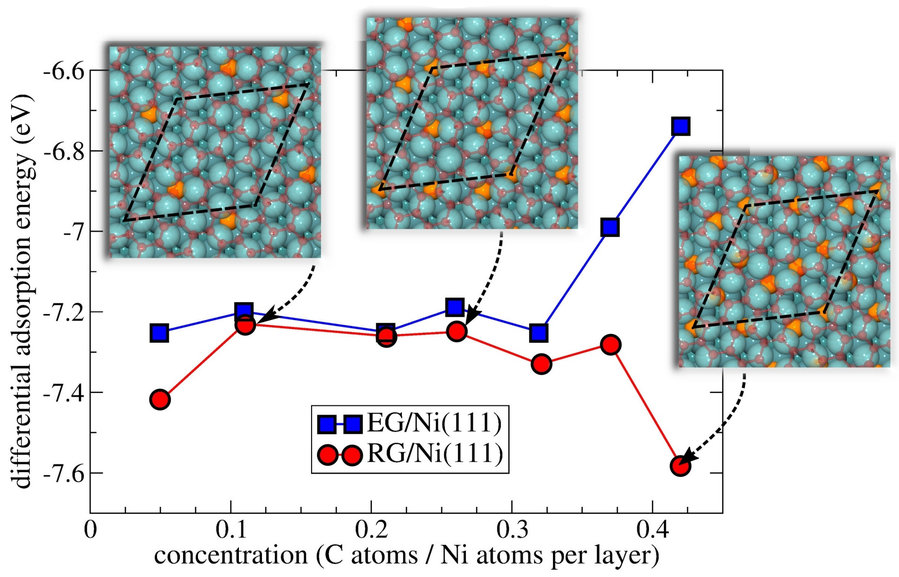
TOWARDS CARBIDE FORMATION

SURFACE SEGREGATION OF Ni-DISSOLVED C



- subsurface o*h* sites are the most stable both in RG and EG for dissolved C
- Surface segregation is an activated process (higher energy barrier under EG)

INCREASING THE CONCENTRATION OF SUBSURFACE C



- C added one-by-one on *oh* sites
- concentration < 0.35: similar chemical potential in EG and RG
- concentration > 0.35: opposite behaviour, under EG further segregation is more difficult

CONCLUSIONS

- EG and RG detached by Ni_2C from the surface (~ free-standing features)
- Ni-dissolved C atoms prefer subsurface octahedral sites
- Carbide formation favored only under RG for thermodynamics and kinetics arguments

CONTACT PERSON

Simone Del Puppo
SIMONE.DELPUPPO@phd.units.it

REFERENCES

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Farnesina
Ministero degli Affari Esteri e della Cooperazione Internazionale

Project funded by a grant from the Italian Ministry of Foreign Affairs and International Cooperation.

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