

Defects in epitaxial graphene on Ni(111): first-principles simulations

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Abstract

The analysis of unprecedented high-resolution scanning tunneling microscopy (STM) images of graphene/Ni(111) shows the presence of different types of defects, mainly due to carbon vacancies and partially filled with trapped Ni adatoms. We have proposed some structural models and verified their reliability on the basis of the energetics and the comparison between observed and simulated STM images, obtained from ab-initio density functional theory calculations. In particular, we have studied in details a triple-vacancy defect with one Ni atom trapped inside, that shows a peculiar dynamical behavior in the interaction with carbon monoxide. We have investigated and characterized also other defects, even more extended, extracting some general trend to predict their stability and their abundance. Preliminary results concerning their activity under the exposure of small molecules of environmental importance have been also obtained.

In collaboration with C. Africh, G. Comelli and L. Patera.

Acknowledgements: Università degli studi di Trieste – Finanziamento di Ateneo per progetti di ricerca scientifica – FRA2015. Computational

resources have been partly obtained through Italian Super-Computing Resource Allocation (ISCRA) grants of the Consorzio Interuniversitario CINECA, partly within the agreement between the University of Trieste and CINECA.

References

- [1] L. L. Patera, C. Africh and G. Comelli, unpublished.
- [2] F. Bianchini, L. L. Patera, M. Peressi, C. Africh and G. Comelli, *J. Phys. Chem. Lett.* **5(3)**, 467-473 (2014).
- [3] G. Prandini. Master thesis in Physics, University of Trieste (2014).
- [4] V. Carnevali, Master thesis in Physics, University of Milan (2015).

Figures

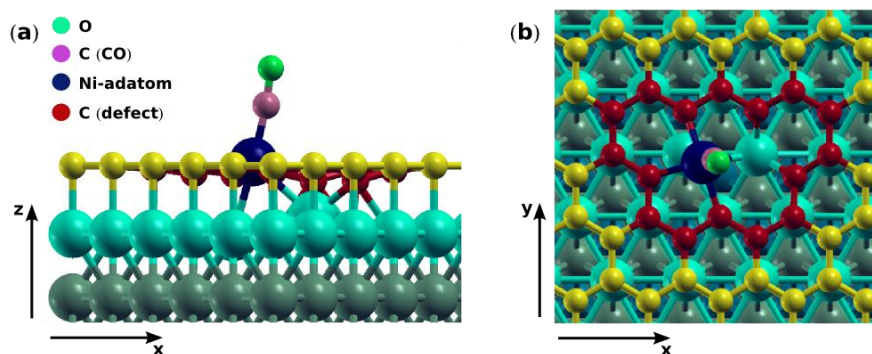


Figure 1. (a) Top and (b) side view of triple vacancy with CO adsorbed on nickel adatom trapped inside the defect. Only the carbon atoms of the defect, CO, nickel adatom and the nickel atoms just below the defect are relaxed.