Growth of nanoparticles on supported graphene: insights from ab-initio calculations

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Abstract

For most practical applications, metal nanoparticles (NPs) need to be supported on a substrate that can act as a deposition template for growing them in regular arrays. This prevents sintering at high temperatures, a process that would deactivate the catalytic devices. The Moire' pattern due to the small lattice mismatch between graphene and Ir(111) support works as an efficient template for the ordered growth of some transition metal NPs [1,2]. With the help of ab-initio calculations performed for adsorption of monomers and small clusters of Cu, Pt, and Ir, we explain the behavior of different metals, predicting results in agreement with the available experimental findings and identifying the criteria for the suitability of a metal to form ordered nanocluster arrays. Moreover, preliminary results indicate that even materials that do not form cluster superlattices can be grown through the application of cluster seeding using properly chosen metals (see Figure 1) [3].

References

[1] A.T. N'Diaye, et al., New J. Phys. **11**, 103045 (2009).

[2] Y. Dedkov, et al., J. Phys.: Condens. Matter. **27**, 303002 (2015)

[3] F. Mohamed, Master Thesis, University of Trieste (2015)

Figures

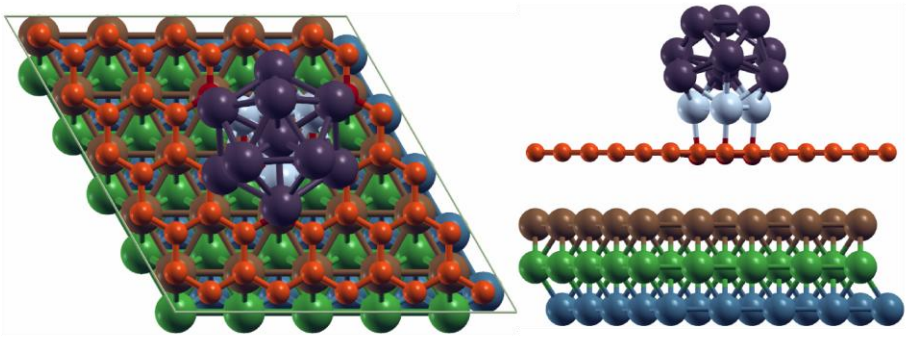

Figure 1. Stick-and-ball model for $Cu_{10}Ir_3$ nanocluster adsorbed in the hcp region on graphene/Ir(111)