The π plasmon of graphene on transition metals in time-dependent density functional theory

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Abstract

While the ground-state electronic properties of graphene grown on transition metals are well established [1-2], a self-consistent approach to the dielectric properties of the interface, and in paticular the energy loss function, is still lacking.
The dielectric properties of graphene adsorbed on the (111) surfaces of nickel and copper is explored using the time-dependent density functional theory within the linear response formalism and the random phase approximation. These cases represent the known prototypes for examining he different interactions between graphene and the substrate it is grown on.
We focus on the graphene derived π plasmon, whose experimental line-shape and dispersion have been recently observed in some electron energy loss spectroscopy (EELS) experiments [3-5].
The predictions of the π plasmon peak are obtained from a perfect graphene sheet placed above 1 to 5-layer slabs of Ni(111) and Cu(111). We draw a link between the measured response of the G/Ni(111) and G/Cu(111) samples and the role of energy-loss processes occurring at different depths of the interface. Our calculations clarify the apparently discordant experimental behaviors of the π plasmon dispersion.

References

[1] G. Bertoni, L. Calmels, A. Altibelli and V. Serin, Phys. Rev. B **71** (2004) 075402.
[2] P.A. Khomyakov, G. Giovannetti, P.C. Rusu, G. Brocks, J. van den Brink and P.J. Kelly, Phys. Rev. B **79** (2009) 195425.
[3] A. Siokoua, F. Ravania, S. Karakalosa, O. Franka, M. Kalbacc, C. Galiotis, Appl. Surf. **257** (2011) 9785-9790.
[4] A. Generalov and Y. Dedkov, Carbon **50** (2012) 183.
[5] A. Cupolillo, N. Ligato and L. Caputi, Carbin **50** (2012) 2588.