Unravelling the mechanisms of giant spin-orbit splitting in graphene on metals

Jagoda Stawińska¹², Jorge I. Cerdá²

¹Department of Solid State Physics, University of Lodz, ul. Pomorska 149/153, Lodz, Poland
²Instituto de Ciencia de Materiales ICMM-CSIC, Cantoblanco, 28049, Madrid, Spain
jagoda.slawinska@uni.lodz.pl

Weak interaction between graphene and metals tends to preserve the graphene’s characteristic Dirac cones almost intact in the band structure. However, recently it has been shown in experiments that even in case of very weak graphene/substrate coupling the presence of a heavy 5d metal can induce giant spin-orbit splitting (SO) of Rashba type in the graphene’s π bands, although the intrinsic SO coupling in graphene is very small. The results of angle- and spin-resolved photoemission spectroscopy have revealed spin-orbit splitting of Dirac cones up to 100 meV for graphene on Ni(111) with an intercalated gold monolayer G/1ML-Au/Ni(111) [1], as well as of about 70 meV for graphene on Pt(111) [2], which offers a large perspective of applications in spintronics. Giant spin-orbit splitting of linear bands has been related to strong hybridization between the graphene’s π and the metals’ d bands at lower binding energies, but the exact mechanism and range of SO remained unclear due to the limitations of the ARPES technique.

We have studied various G/Pt(111) Moiré phases as well as a realistic G/1ML-Au/Ni(111) interface via large-scale DFT calculations (including SO coupling [3]) coupled to Green’s functions. The simulations of pseudo-ARPES maps show SO splittings in G/Pt(111) as large as 200 meV for specific energy ranges and directions in the Brillouin zone. Giant SO splitting occurs in the regions where graphene’s π and metals’ d bands cross and couple to each other within the same spin orientation (see Figure below) [4]. The effect of spin-orbit splitting is preserved over a considerable range around the point of crossing, but its value decreases rapidly becoming smaller than 20 meV close to the Fermi level.

In contrast, for G/1ML-Au/Ni(111) we have obtained values for the SO splitting always smaller than 30 meV, which correlates well with the low SO split detected in earlier experiments [4]. This suggest that the recent giant SO obtained for this system is not induced solely by hybridization with bands of the metallic substrate. Our calculations revealed other possible factors responsible for large SO such as the presence of Au adsorbates.

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**References**


**Figures**

![Figure 1](image)

*Unfolded and graphene-projected DOS (k, E) along direction (a) ΓK for 3x3p phase and (b) perpendicular to ΓK for 2x2Γ phase of G/Pt(111). To enhance the contrast the difference of spin components has been plotted. Blue color represents the regions of zero SO splitting.*