Surface on Surface. Survey of the Monolayer Gold-Graphene Interaction from Au12 and PAH via Relativistic DFT Calculations

Muñoz-Castro A.

Gomez T.

Carey D.M.

Miranda-Rojas S.

Mendizabal F.

Zagal J.H.

Arratia-Perez R.

Gold-graphene interaction at the interface is evaluated through different polyaromatic hydrocarbons (PAH), accounted by C6H6, C24H12, C54H16, and C96H18, focusing into different energetic terms related to the overall interaction. Our results characterize the neutral gold-PAH interaction nature with 45% of dispersion character, 35% of electrostatic, and 20% of covalent character, suggesting that moderate van der Waals character is mostly involved in the interaction, which increases according to the size of the respective PAH. The resulting surface charge distribution in the graphene model is a relevant parameter to take into account, since the ability of the surface charge to be reorganized over the polycyclic structure in both contact and surrounding regions is important in order to evaluate interactions and different interacting conformations. Our results suggest that for a Au12 contact surface of radius 4.13 Å, the covalent, electrostatic and dispersion character of the interaction are effectively accounted in a graphene surface of about 6.18 Å, as given by circumcoronene, depicting a critical size where the overall interaction character can be accounted.