

# Surface on Surface. Survey of the Monolayer Gold-Graphene Interaction from Au<sub>12</sub> and PAH via Relativistic DFT Calculations

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© 2016 American Chemical Society. Gold-graphene interaction at the interface is evaluated through different polyaromatic hydrocarbons (PAH), accounted by C<sub>6</sub>H<sub>6</sub>, C<sub>24</sub>H<sub>12</sub>, C<sub>54</sub>H<sub>16</sub>, and C<sub>96</sub>H<sub>18</sub>, 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 Au<sub>12</sub> contact surface of radius 4.13 Å, the covalent, electrostatic and dispersi