Retained Carrier-Mobility and Enhanced Plasmonic-Photovoltaics of Graphene via ring-centered η⁶-Functionalization and Nanointerfacing

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Binding graphene with auxiliary nanoparticles for plasmonics, photovoltaics, and/or optoelectronics, while retaining the trigonal-planar bonding of sp² hybridized carbons to maintain its carrier-mobility, has remained a challenge. The conventional nanoparticle-incorporation route for graphene is to create nucleation/ attachment sites via "carboncentered" covalent functionalization, which changes the local hybridization of carbon atoms from trigonal-planar sp² to tetrahedral sp³. This disrupts the lattice planarity of graphene, thus dramatically deteriorating its mobility and innate superior properties. Here, we show large-area, vaporphase, "ring-centered" hexahapto (η^6) functionalization of graphene to create nucleation-sites for silver nanoparticles (AgNPs) without disrupting its sp² character. This is achieved by the grafting of chromium tricarbonyl [Cr(CO)₃] with all six carbon atoms (sigma-bonding) in the benzenoid ring on graphene to form an $(\eta^{6}-graphene)Cr(CO)_{3}$ complex. This nondestructive functionalization preserves the lattice continuum with a retention in charge carrier mobility (9% increase at 10 K); with AgNPs attached on graphene/n-Si solar cells, we report an ~11fold plasmonic-enhancement in the power conversion efficiency (1.24%).

References

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Figure 1: Schematic of hexahaptofunctionalized graphene [(η⁶graphene)Cr(CO)₃]. Raman spectra obtained by averaging the circle area of graphene without (blue line) and with hexahapto functionalization (red line).



Figure 2: FESEM images of η^{6} -functionalized graphene with silver nanoparticles. J vs. V characteristics curves of solar cells with AM 1.5G illumination, the inset is an enlarged view of G/Si and η^{6} -G/n-Si.