

Graphene nanoribbon electrical decoupling from metallic substrates

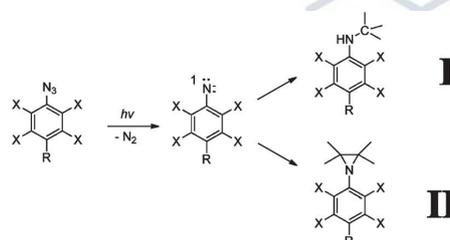
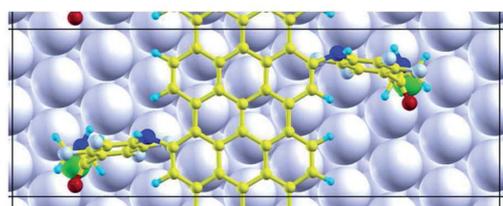
Ivo Borriello¹, Giovanni Cantele² and Domenico Ninno^{1,2}

¹ Università di Napoli "Federico II", Dipartimento di Scienze Fisiche, Complesso Universitario Monte Sant'Angelo, Via Cintia, I-80126 Napoli, Italy

² CNR-SPIN, Complesso Universitario Monte Sant'Angelo, Dipartimento di Scienze Fisiche, Via Cintia, I-80126 Napoli, Italy

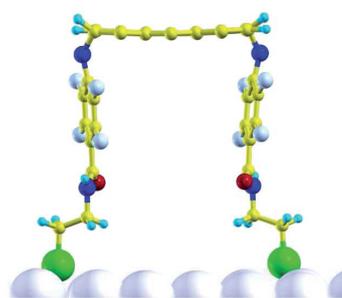
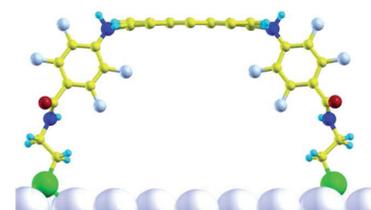
NANOSCALE 5, 291 (2013)

We address the structural and electronic properties of graphene nanoribbons (GNRs) covalently immobilized on a metallic substrate by means of an organic layer. The GNR–organic layer and organic layer–metal interfaces can be thought of as constituents of a nanodevice and have been accurately studied using large-scale density functional theory calculations. Our results demonstrate the possibility of combining nanopatterned metal–organic layer substrates with selected GNRs to obtain well ordered and stable structures while preserving the GNR energy band gap, an essential requirement for any switching nanodevice.



(a)

(b)



(c)

(d)

Fig. (a) Top view of an armchair GNR covalently linked to the Au (111) surface through PFPA (the in-plane supercell is also represented). (b) Schematic view of the two possible PFPA–GNR link mechanisms (see text): insertion (I) and addition (II). The side views of the resulting Au–PFPA–GNR systems are given in (c) and (d), respective