# Electron and Optical Spectroscopies of Graphene Nanoribbons on Au(111)

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Graphene nanostructures have striking properties related to their lateral confinement that can open a band gap and induce a semiconducting behavior with controlled quantum states and a variety of peculiar width- and edge-related phenomena depending on the details of the atomic structure. Radically new functionalities can thus be designed, far beyond those expected from extended graphene systems or conventional semiconductors. Key features connected to the tunability of electronic and optical properties as a function of structural parameters, e.g. width and edge structure of graphene nanoribbons (GNR), have been predicted theoretically (see e.g. [1]); however, only recently atomic control of GNR geometry was demonstrated on Au(111) susbtrate [2], thus opening the way for their experimental investigation and exploitation.

In this work we combine cutting edge theoretical and experimental techniques to study the electronic and optical properties of ultranarrow atomically precise GNRs on Au substrate. Band structures and optical spectra were computed from first principles for isolated GNRs, fully accounting for many-body effects; the presence of the substrate was included within a classical image charge model for the screened Coulomb interaction. Our findings show that the metallic substrate induces a giant reduction of the energy gap as compared to the isolated system, bringing the electronic gap from 3.7 ± 0.1 eV in gas phase to 2.3-2.7 eV on Au(111), in excellent agreement with STS measurements [3]. On the contrary, the position of the optical peaks remains unaltered, reproducing the experimental observations from reflectance difference spectroscopy (RDS) [4]. This combined approach allows us to show that ultranarrow GNRs have fully anisotropic optical properties dominated by excitonic effects that sensitively depend on the exact atomic structure. For the considered GNRs, ab initio calculations also reveal an absorbance of more than twice the one of graphene for linearly polarized light in the visible range of wavelengths [5].

**References**

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