



Mercoledì 2 dicembre alle ore 15:00

Nell'aula Diagonale del dipartimento di Chimica,
via Giuria 7

il dott. Andrea Ferretti

ricercatore presso l'Istituto di
Nanoscienze del CNR, sede di Modena

terrà il seminario

**"Electron and Optical Spectroscopies of Graphene
Nanoribbons on Au(111): Insights from Ab-Initio
Calculations"**

Abstract:

Narrow graphene nanoribbons (GNRs) exhibit substantial electronic band gaps and optical properties expected to be fundamentally different from the ones of their parent material graphene. Unlike graphene the optical response of GNRs may be tuned by the ribbon width and the directly related electronic band gap.

In this work we perform ab initio calculations and compute quasiparticle energies and optical properties of GNRs within the so-called GW-BSE scheme. We focus on a specific armchair nanoribbon (7-AGNR). The presence of the substrate is accounted for by means of a classical image charge model for the screened Coulomb interaction. Our findings show that the metallic substrate induces a significant reduction of the energy gap as compared to the isolated 7-AGNR, bringing the GW gap from 3.7 ± 0.1 eV to 2.3-2.7 eV on Au(111). On the contrary, the position of the optical peaks remains unaltered. Our results are in very good agreement with the experimental values obtained by STS, ARPES, and differential reflectance data, indicating that this scheme can provide quantitative predictions for electron and optical spectroscopies of nanoribbons on weakly coupled substrates such as Au.

Contatto:

Lorenzo Maschio

lorenzo.maschio@unito.it