Growth, characterization and perspectives of applications of novel 2D carbon-based materials

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Novel 2D carbon-based materials, as graphynes and graphdiynes, formed by atoms with both sp- and sp2-hybridization [1], display interesting structure-properties relationship that make them suitable for different applications, including nanoelectronics, catalysis, photo-conversion and water splitting [2]. Exploiting a bottom-up on-surface synthesis approach, based on temperature-driven assembly of molecular precursors, it is possible to design different π-conjugated networks with tailored structural, electronic and optical properties [3]. In view of their applications is of fundamental importance to understand how the structure and the growth conditions affects the final properties and define protocols for the fabrication of extended 2D layers and for their controlled manipulation.

After a brief overview of the technological relevance of these 2D materials, we present a multidisciplinary characterization of hybrid sp- sp^{2-} 2D systems obtained by on-surface synthesis of brominated molecular precursors on metal surfaces. By combining *ab initio* theoretical calculations and different experimental techniques, such as Scanning Tunneling Spectroscopy and Microscopy (STS and STM), Raman spectroscopy and Angle-Resolved Photoemission (ARPES) we are able to give a thorough description of nanoscale 2D networks [4-9]. In particular we analyze the evolution of the structural, electronic and vibrational properties during the different stages of the formation, passing from the as deposited metallorganic network to pure sp-/ sp^2- nanostructures upon annealing, and we show the effect of the substrate coupling on their electronic properties.

References

[1] Y. Fang, Y. Liu, L. Qi, Y. Xue and Y. Li, Chem. Soc. Rev 51, 2681 (2022).
[2] H. Yu, Y. Xue and Y. Li, Adv. Mater. 31, 1803101 (2019).
[3] C. S. Casari et al. MRS Communications 8(2), 207-219 (2018).
[4] Fratesi, G. et al., Materials 11, 2556 (2018).
[5] Rabia, A. et al., Nanoscale 11, 18191 (2019).
[6] Rabia, A. et al., ACS Appl. Nano Mater. 3, 12178 (2020).
[7] S. Achilli et al. 2D Materials 8 044014 (2021).
[8] S. Achilli et al. Phys. Chem. Chem. Phys. 24, 13616-13624 (2022).
[9] P. D'Agosta, S. Achilli et al. arXiv:2404.06896

Figures

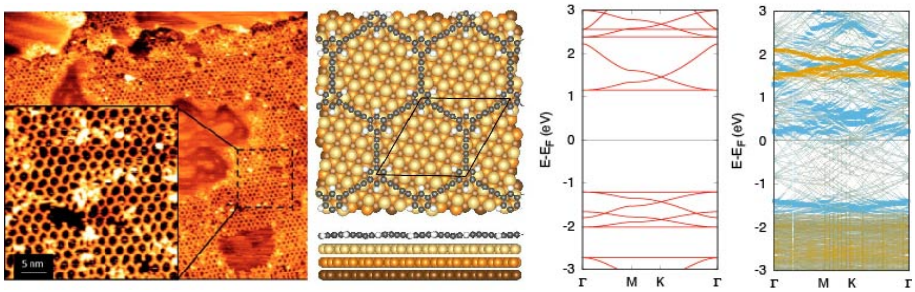

Figure 1: STM image and theoretical model of h-GDY/Au(111). On the left: calculated bandstructure of the freestanding and supported network.