Friday Materials Science Colloquia

Friday, January 27th 2023, 12 p.m.
Seminar room, U5 Building – via Roberto Cozzi 55, Milano

Lecturer: **Chiara Ferrara**

Title: **MXene compounds as anode for sodium-ion batteries: structure, defects, electrochemical behavior**

MXenes are a new class of layered materials characterize by some unique structural and functional features, making them appealing for the use as electrodes in energy storage devices such as rechargeable batteries and supercapacitors [1]. Electrochemical performance of MXenes have been widely investigated in the recent years, but, at the same time, their structure is still not completely resolved [1,2]. Aim of this project was the investigation of the structure of the $Ti_3C_2T_x$ with T = F, O, OH, the most common MXene composition and the one showing the best performance when tested as electrode in sodium ion batteries. Due to the complexity of the system, the combination of different techniques (neutron diffraction, XAS, XPS) was necessary to combine different information and, also considering the precursor compound (the MAX phase Ti_3AlC_2) it was finally possible to build a structural model fitting the experimental data and to correlate peculiar structural features with the observed electrochemical behavior [3].

References:
[1] C. Ferrara et al, Current Opinion in Electrochemistry 29, 100764 (2021)
[2] A. Gentile et al, Small Methods 4, 2000314 (2020)
[3] C. Ferrara et al., Nano Letters 21, 8290-8297 (2021)

Lecturer: **Emilio Scalise**

Title: **Group IV allotropes: challenges and opportunities down the road for silicon-based technology**

The boost of the new technologies crucially requires new materials providing better performance and expanding the range of applications of traditional semiconductors. Still, the effective exploitation of the new materials faces the integration into the current Si technology. Using silicon itself, or other group-IV elements, but in the form of nanostructures and/or even in different crystalline phases may facilitate the integration of diverse and advanced functionalities in a single chip. This was the basic idea of the initial theoretical studies of a single layer of silicon, so called silicene, which was predicted to manifest massless Dirac fermions, similar to graphene. Soon silicene was synthesized on Ag substrate [1], but experimentally it was not really behaving like graphene [2], because of two main weaknesses: metastability and interfaces. To overcome these problems, non-metallic substrates were investigated, particularly focusing on layered compounds, such as the transition metal dichalcogenides. These studies led to the growth of silicene on MoS_2 [3]. A considerable number of metastable polytypes of group IV elements have been also investigated and obtained in the form of nanoparticles (0D), nanowires (1D), or even bulk-like structures, by using different approaches, spanning from wet chemistry strategies to pressure-induced phase transition. All of these attempts to exploit the group IV allotropes suffer from similar problems that were bedevilling the 2D structure, and a few of them will be briefly discussed.

References:
[1] P. Vogt et al., PRL 108, 155501 (2012)
[2] E. Cinquanta, E. Scalise et al., J. Phys. Chem. C 117, 16719 (2013)
[3] D. Chiappe, E. Scalise et al., Adv. Mater. 26, 2096 (2014)