



Giovedì **27 febbraio 2025** alle ore **11:30** presso l'aula **E** del DiSC

il Dr. Luca Tortora

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terrà il seminario dal titolo:

Decoding graphite intercalation mechanisms for next-generation ion batteries and graphene production: a combined low-energy ion bombardment and DFT approach

Graphite intercalation is a multifaceted process that plays a pivotal role in advancing energy storage technologies. In this seminar, I will present our integrated experimental and theoretical approach to decoding the early stages and beyond of ion intercalation in highly oriented pyrolytic graphite (HOPG). Using low-energy ion bombardment experiments combined with in situ techniques such as electrochemical atomic force microscopy (EC-AFM) and scanning tunneling microscopy (STM) we have observed the formation of discrete nano-protrusions on the basal plane of HOPG. These features highlight how localized surface deformations are initiated during early intercalation. It will be shown how complementary density functional theory (DFT) calculations, though not the main focus, support our experimental observations by indicating that initial intercalation likely involves the incorporation of one or two ions, sufficient to trigger these nano-scale deformations without causing extensive damage deeper in the structure. Chemical imaging experiments will be presented to illustrate the mechanisms of basal-plane intercalation, a process that remains less understood than edge intercalation. I will also show how we sequentially sputtered away the graphite basal layers to obtain the concentration profile of the intercalated electrolytes. We compared the effects of different ion sputtering sources (Cs^+ and Ar gas cluster) at various energies to minimize morphological alterations and chemical modifications (e.g., the formation of graphite oxide) in the graphitic electrodes. This combined experimental-theoretical study provides new insights into the interplay between ion intercalation, surface defect formation, and subsequent exfoliation processes in graphitic materials.

La presenza della S. V. sarà molto gradita

Il Direttore del Dipartimento