Title: An atomistic incursion into the 2D world: when simulations meet material reactivity

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Abstract

The last decade witnessed the crystallization of the interest of the scientific community for the discovery, the development, and the growth of two-dimensional materials. Among the technological opportunities they offer, their exceptional electronic properties make them promising candidates to challenge the reign of Silicon in the development of future CMOS nodes.

However, the difficulty to synthesize high mobility semi-conducting materials, the high occurrence of intrinsic defects, adhesion issues and their sensitivity to the different integration steps used in the building process of a transistor are still roadblocks that need to be ironed out to unleash their potential. This is needed to enable the actual demonstration of high-performance devices with synthetic materials. Therefore, gaining insights into mechanisms that link their reactivity and their chemical environment to their properties is key.

In this talk, I will discuss how atomistic simulations can be used to gain the fundamental understanding needed to meet these challenges. I will illustrate how the predictivity of first-principle simulations can be used to evaluate the material evolution during different chemical events taking place in a CMOS process, going from the Metal Organic Chemical Vapor Deposition (MOCVD) synthesis of MoS_2 and WS_2 material, the deposition of a dielectric or a metal. Finally, I will also discuss how the interaction of some of the by-products generated during the synthesis of the material leads to the degradation of silicon wafers.