Joint theoretical and experimental characterization of 2D materials heterostructures towards an improved growth efficiency

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Combining 2D materials forming heterostructures is a well recognized strategy to enlarge the realm of their properties and introduce new functionalities [1]. Nevertheless their controlled growth is challenging and monitoring the structure-properties relationship in the experimental synthesis with the support of a theoretical analysis is fundamental to define growth protocols.
We present two joint experimental and theoretical study of supported 2D materials whose growth can be controlled and eventully improved by appropriately tailoring the substrate. The first one is a vertical heterostructure formed by silicene on silver, which is usually characterized by different phases and domains that hinder the transfer and the application in electronic transport devices. We show that by engineering the silicene/silver interface through the inclusion of Sn atoms, forming Ag2Sn alloy or a thin stanene buffer layer, a single and well determined phase can be achieved and stabilized: a 4x4 reconstruction via Sn decoration and a $\sqrt{3}\times\sqrt{3}$ for the buffered interface, respectively [2,3]. We provide a detailed ab initio theoretical characterization supporting the experimental measurements as proof of this evidence.
The second example is represented by organometallic networks obtained through on-surface synthesis of molecular precursors on metal surfaces. In such temperature-assisted process the substrate assumes a pivotal role due to its catalytic effect. Through a joint theoretical and experimental characterization, including DFT calculations, Raman, STM and ARPES experiments, we analyze the growth of a organometallic network on different Au surfaces demonstrating how the choice of the metal surface impacts on the efficiency of the ordered growth and on the final properties [4, 5, 6].

References

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