Group IV two-dimensional materials : Novel electronic and structural properties

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There has been much progress in the synthesis and characterization of nanostructures however; there remain immense challenges in understanding their properties and interactions with external probes in order to realize their tremendous potential for applications (molecular electronics,light harvesting and emitting nanostructures). Here we review the recent advances within density-functional based schemes to describe spectroscopic properties of low dimensional structures. We will star by reviewing the work done over the last years on on carbon-based pure and hybrid nanostructures: from nanotubes to graphene to C-B-N heterostructures. We will review their thermodynamical stability, mechanical, electronic, structural and optoelectronic properties. We will use those systems as test-bed to illustrate the predictive power of the first-principles techniques we have developed over the last years to characterize and predict properties of materials at the nanoscale. The success of the theoretical predictions that were confirmed experimentally open the path towards the recent work we conducted on other two-dimensional materials based on Si, Ge and Sn (as well as transition metal dichalcogonides that would not be discussed in the present talk). In this context we predicted two new thermodynamically stable single and multi- layered-phases of silicon which exhibit strong directionality in the electronic and structural properties. As compared to silicon crystal, they have wider indirect band gaps but also increased absorption in the visible range making them more interesting for photovoltaic applications. Moreover, the intrinsic two-dimensional confinement and strong electron-phonon coupling make them a candidate material for thermoelectricity and superconductivity. These stable phases consist of intriguing stacking of dumbbell (DB) patterned silicene layers having trigonal structure with $\sqrt{3}\times\sqrt{3}$ periodicity of silicene. We propose a new mechanism for explaining the spontaneous and consequential formation of $\sqrt{3}\times\sqrt{3}$ structures from 3×3 structures on Ag substrate. We show that the $\sqrt{3}\times\sqrt{3}$ reconstruction is mainly determined by the interaction between Si atoms and have weak influence from Ag substrate. The proposed mechanism opens the path to understanding of multilayer silicon and silicites. We extended those studies to Ge and Sn. For the case of Ge, we showed that single and multi--layer germanium grow on a gold (111). Its growth bears strong similarity with the formation of silicene layers on silver (111) templates. One of the phases shows a clear, nearly flat, honeycomb structure. Thanks to thorough synchrotron radiation core- level spectroscopy measurements and advanced Density Functional Theory calculations we identify it to a $\sqrt{3}x\sqrt{3}R(30^{\circ})$ germanene layer in

coincidence with a $\sqrt{7}x\sqrt{7}R(19.1^{\circ})$ Au(111) supercell. For the case of Sn, we predict from the first-principles calculations that the stanene with dumbbell units (DB) is a fully stable two-dimensional (2D) topological insulator with inverted bands around the Γ point and its band-gap can be tuned by compressive strain. The quantum anomalous Hall effect, Chern half metallicity and topological superconductivity are possible to be observed in DB stanene.

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