## Silicene on insulating substrates and in heterostructures

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Abstract

In the quest of other two-dimensional materials beyond graphene a large attention has been devoted to silicene. Up to now, preserving the properties of silicene when it is deposited on a substrate has proven to be a hard task. A much studied substrate is Ag(111), with which, however, silicon significantly interacts [1]. Recently, Al2O3(0001) has been proposed as a viable substrate to grow silicene, in view of its insulating behaviour [2].

We studied the system silicene/Al2O3(0001) by means of DFT calculations of its structural, electronic and optical properties, with the aim of interpreting the measured optical conductivity of silicon nanosheets recently synthesized by molecular beam epitaxy [3].

Another possibility to preserve the properties of silicene, as suggested for various 2D materials, is the design of van der Waals heterostructures. The partner of silicene in such an heterostructures might be a monolayer of Al2O3, that has been predicted to be stable in an hexagonal Kagome lattice [4]. We show by DFT, GW and BSE calculations [5] that the honeycomb buckled structure of silicene is negligibly affected by the interaction with a monolayer of Al2O3, so that the electronic band structure shows unperturbed cones with massless Dirac fermions embedded by Al2O3-derived bands. As a consequence, also the optical properties of the heterostructure show the preservation of the infrared universal limit characteristic of freestanding silicene and a quantized absorbance occurs for stacking of multilayers.

**References:**

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