

SILICENE ON INSULATING SUBSTRATES

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The continuous interest raised by the ever-expanding number of peculiar properties of graphene has stimulated the birth of many parallel research paths devoted to the exploration of other two-dimensional materials and, among them, to group-IV based nanomaterials and to silicene, in particular.

Although many of its interesting properties derive from its similarity with graphene, e.g. the electronic and optical ones, other characteristics are peculiar of silicene and are connected with its buckled structure. As an example, the buckling affects silicene phonon spectrum and is at the origin of a much lower thermal conductivity than the one of graphene, making silicene appealing for thermoelectric applications. The mixed sp²-sp³ hybridization that characterizes silicene makes it much more reactive than sp²-hybridized graphene. This can be exploited in silicene use as a molecule sensor and as a trap to catch harmful molecules.

At the same time this reactivity is at the origin of the difficulty of preserving the properties of silicene when it is deposited on a substrate. A much-studied substrate is silver, with which, however, silicon significantly interacts. Recently, Al₂O₃(0001) has been proposed as a viable substrate to grow silicene, in view of its insulating behaviour. 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 (MBE).

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. We show by calculations 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.