Electronic Supplementary Information

Scanning tunneling microscopy and Raman evidences of silicene nanosheets intercalated into graphite surface at room temperature

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Abstract:

Highly oriented pyrolitic graphite (HOPG) is an inert substrate with a structural honeycomb lattice, well suited for the growth of two-dimensional (2D) silicene layer. It was reported that when Si atoms are deposited on HOPG surface at room temperature, they arrange in two configurations: silicene nanosheets and three dimensional clusters. In this work we demonstrate, by using scanning tunneling microscopy (STM) and Raman spectroscopy, that a third configuration stabilizes in the form of Si 2D nanosheets intercalated below the first top layer of carbon atoms. The Raman spectra reveal a structure located at 538 cm^{-1} which we ascribe to the presence of sp^2 Si hybridization. Moreover, the silicon deposition induces several modifications in the graphite D and G Raman modes, which we interpret as an experimental evidence of the intercalation of the silicene nanosheets. The Si atom intercalation at room temperature takes place at the HOPG step edges and it detaches only the outermost graphene layer inducing a strong tensile strain mainly concentrated on the edges of the silicene nanosheets. Theoretical calculations of the structure and energetic viability of the silicene nanosheets, of the strain distribution on the outermost graphene layer and its influence on the Raman resonances support the STM and Raman observations.

Fig. S1: Raman spectra deconvolution with Voigt curves. Raman peak parameters are reported in Table S1 and Table S2. The Voigt deconvolution reveals the doubling of the D and G peaks, showing an additional peak for each mode. In Table S2 presents the parameters of the Raman modes of the sp^3 silicon (517 cm^{-1}) and of silicene located at 538 cm^{-1}

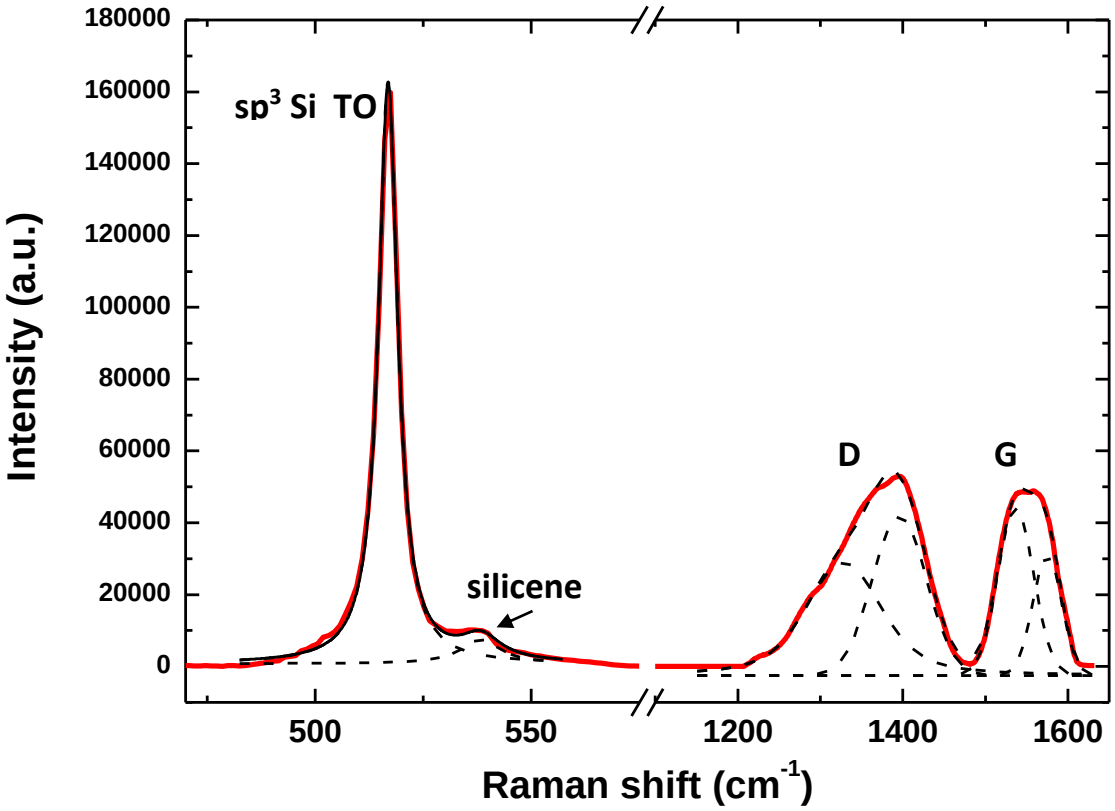

Table S1

	Before Silicon Deposition			After Silicon Deposition		
	Raman Shift (cm^{-1})	FWHM (cm^{-1})	Intensity x 10^5 (cps)	Raman Shift (cm^{-1})	FWHM (cm^{-1})	Intensity x 10^5 (cps)
G mode	1579	15	25.6	1575	41	14.8
				1536	51	25.3
D mode	1359	43	6.2	1328	108	43.9
				1395	77	36.4

Table S2

	Raman Shift (cm^{-1})	FWHM (cm^{-1})	Intensity x 10^5 (cps)
Si TO	517	5.4	13.7
Silicene	538	11.2	1.2