Molecular adsorption on Dumbbell Silicene

L. Florean[1, 2], H. Cruguel[1], Y. Borensztein[1], R. Bernard[1], F. Bournel[2], G. Prevot[1]

[1] *Institut des NanoSciences de Paris, Sorbonne University, Paris, France*
[2] *Laboratoire de Chimie Physique – Matière et Rayonnement, Sorbonne University, Paris, France*

laurita.florean@insp.jussieu.fr

Following graphene discovery, 2D materials attracted rising attention due to their remarkable properties. Among them, silicene has been particularly studied as Si is essential in semi-conductor industry. Silicene presents an electronic structure very similar to the one of graphene [1], but is more sensitive to chemical environment. The possibility of tuning the electronic properties of silicene by molecular adsorption associated with the 2D geometry makes it a promising candidate for highly sensitive molecular sensors.

We have recently proven the existence of Dumbbell Silicene (DBSi) obtained by thermal evaporation of Si onto Ag(110) at 200°C [2]. It shows a low density of adatoms, on top of Si atoms of the silicene layer (Fig. 1b), forming DB units. Adsorption of molecules onto these sites is expected to open a small gap in the electronic structure, while preserving the overall silicene band structure [3].

Using operando STM, we have followed the evolution of DBSi/Ag(110) upon exposure to various molecules (O_2, triethylamine (TEA), NH_3). The adsorption is characterized by the strong interplay between physisorption and dissociative chemisorption. While oxygen easily dissociate at room temperature, TEA and NH_3 have a much lower probability to dissociate. We have followed NH_3 adsorption at various temperatures from 120K to 300K. Our results show that NH_3 has only a weak tendency to dissociate on DB sites at room temperature, on contrary to what is observed after low temperature adsorption, for which a marked preference for adsorption on DB sites is observed (see Fig. 1c).

Our results open interesting perspective for tuning the electronic properties of a silicene layer through selective adsorption on DB sites.

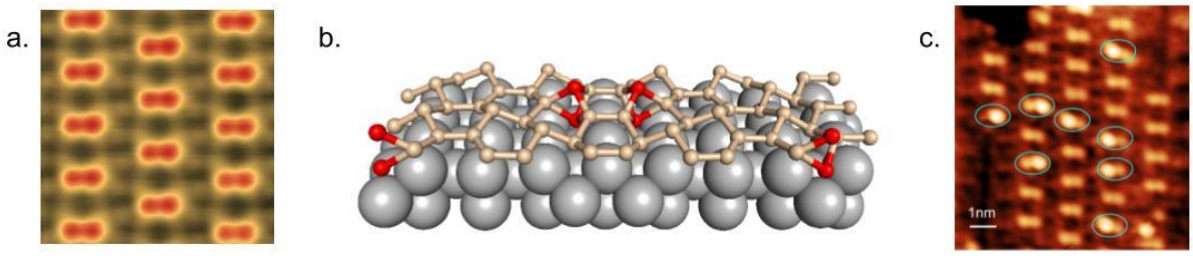

Fig. 1. a) STM image of the periodic DBSi mono-layer (5x5 nm^2) on Ag(110). b) schematic of silver substrate (gray) with the silicene layer above and the DBSi (highlighted in red). c) STM images of NH_3 adsorbed on Dumbbell Silicene at 123K (Height of the DBs ≈ 85pm; height of the NH_3 adsorbed on DB ≈ 50pm)

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