Molecular adsorption on Dumbbell Silicene

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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 its properties 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) which shows a low density of adatoms, on top of Si atoms of the silicene layer. 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].

For this purpose, we have studied ammonia adsorption on DBSi in the 10^{-10} mbar - 10^{-7} mbar and 120 K – 300 K pressure and temperature ranges. Using operando STM, we have identified the mechanisms of NH_3 adsorption at the atomic scale. While NH_3 molecules preferentially physisorb in-between the DB atoms, we show that they preferentially dissociatively chemisorb on the DB atoms. These observations pave the way to the chemical functionnalization of a silicene layer.

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