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Exploring Silicene mono- and multilayers of Silicene and their oxidation with soft X-ray spectroscopy and DFT calculations

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2012 brought the first reports of a new member of the 2D material family: a hexagonal honeycomb of Si atoms deposited on the Ag(111) surface called “silicene”[1]. The characteristics and stability of freestanding silicene had previously been theoretically explored [2], and there was a strong push to determine if the epitaxial sheets possessed the promising qualities of their hypothetical freestanding counterparts. Initially, ARPES experiments were thought to indicate that epitaxial silicene had a gapped Dirac cone in its electronic structure [1], as would be expected of freestanding silicene with a broken inversion symmetry. This enticing result, however, would be later overturned through a combination of experimental and theoretical techniques [3-5], and it would eventually be concluded that the epitaxial silicene sheet was in fact metallic with a strong cohesion to the underlying Ag(111) face. However, this conclusion would prove controversial [6,7], as the ambiguity of the ARPES data left some room for interpretation as to whether specific electronic features belonged to the epitaxial Si, the Ag substrate, or represented a hybridization between the two.

Soft X-ray emission and absorption spectroscopy (XES and XAS) are synchrotron-based experimental techniques for directly probing the (element-specific) partial density of electronic states (PDOS) in the valence and conduction bands of a material. When performed at the Si L_{2,3} emission and Si 2p absorption edges, XES and XAS allowed us to unambiguously show that the Si valence and conduction states were continuous across the Fermi energy; i.e. that the silicene overlayer was indeed metallic [3]. However, for the material to be of use, it must be isolated from the substrate. One suggested way of achieving these characteristics is to produce a multilayer of silicene on the Ag(111) surface. However, other reports insist that bilayers and multilayers are inherently unstable, collapsing into bulk Si nanocrystals shortly after the monolayer deposition is complete [8].

Our DFT calculations [9] predict a stable, AA-stacked silicene bilayer on Ag(111) that corresponds nicely to the scanning tunnelling microscopy (STM) bilayer observations. Unfortunately, these same DFT calculations predict a similar electronic structure as that of the monolayers, namely metallic and bound to the Ag(111). However, our XES and XAS measurements indicate a transition to bulk, sp³-hybridized Si beginning shortly after the completion of a monolayer, supporting the low-energy electron microscopy study that first suggested the nucleation of the silicene sheets to bulk crystals [9]. Finally, we will discuss our recent study in which we explore how Silicene oxidizes [10].

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