

The work on the isolated protein was concluded during the time of the evaluation of the proposal, then we focused directly on the understanding of substrates where we wanted to deposit the proteins and study their interactions. While we studied various two-dimensional (2D) materials as candidate substrates we encountered several opportunities that eventually led to three major publications. We summarize these three results below.

In the first [study](#), the structural evolution of silicene, the silicon counterpart of graphene, in the presence of oxygen atoms was investigated. We discovered that as the oxidation proceeds, silicene transforms into silicatene which can be considered as the 2D counterpart of the quartz crystal. Our calculations revealed that, similar to the quartz crystal, silicatene also has a high piezoelectric coefficient which means that the structure of silicatene changes significantly when electric field is applied. Moreover, we have shown that silicatene is an auxetic material with a negative Poisson ratio. This means that unlike ordinary materials, when silicatene is pulled in one direction it also widens in the perpendicular direction. This is due to the reentrant Si-O bonds that form the atomic structure of silicatene (see Figure 1).

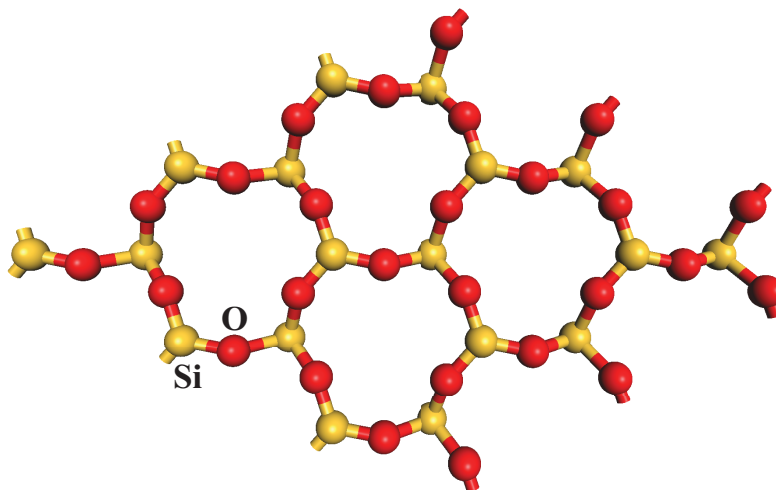


Figure 1: The atomic structure of silicatene. The reentrant Si-O bonds makes silicatene an auxetic material.

The second [study](#) involved understanding of the structure of silicene that was recently synthesized on Ag(111) substrates. The experiments reported various reconstructions on silicene surface and two of them were reported the most. The atomic structure of the first one composed of 3×3 reconstructed silicene matched by 4×4 supercell of Ag(111) surface was very well understood. The second one, on the other hand, was composed of $\sqrt{3} \times \sqrt{3}$ silicene with 5 % lattice contraction and bright spots arranged in a honeycomb lattice as observed in the scanning tunneling microscopy (STM) measurements. There were no models that could explain the lattice contraction or the honeycomb STM pattern. To understand the emergence of this latter reconstruction we started from silicene and added new silicon atom. We discovered that this leads to formation of a dumbbell unit that is composed of two silicon atoms sitting 1.3 \AA below and above silicene while being connected to the same three silicon atoms (see Figure 2). Our calculations have shown that as the process of adding silicon atoms is continued, silicene on Ag(111) surface is transformed into the so called honeycomb dumbbell silicene structure (HDS) that reproduces both the 5 % lattice contraction and the $\sqrt{3} \times \sqrt{3}$ honeycomb STM pattern observed in experiments.

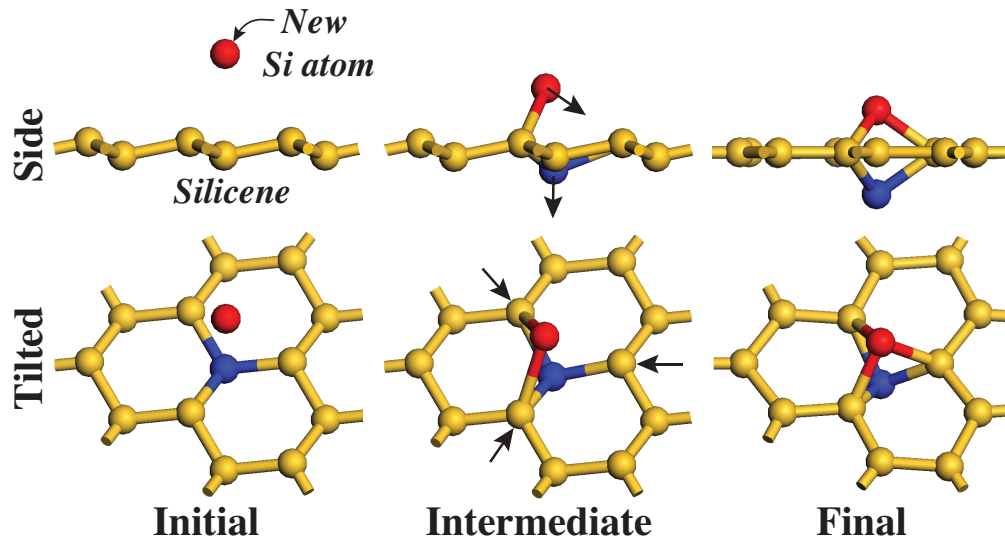


Figure 2: Formation of dumbbell units. Adding an extra silicon atom to silicene leads to the formation of so called dumbbell units.

In the third [study](#) we tried to explain recent experiments on synthesis of multilayer silicene. The contracted $\sqrt{3}\times\sqrt{3}$ reconstruction and the honeycomb STM pattern were observed also on the surfaces of these multilayers of silicene. We started with the HDS structure that successfully explained the experiments on monolayers and added more silicon atoms to extend it to the multilayer silicene case. This led us to a new layered allotrope of silicon that we named silicite. Due to the layered nature of silicite, its properties are anisotropic in the in plane and out of the plane directions. Our calculations have shown that silicite can absorb more visible light compared to cubic diamond silicon which makes it a potential candidate for photovoltaic applications (see Figure 3).

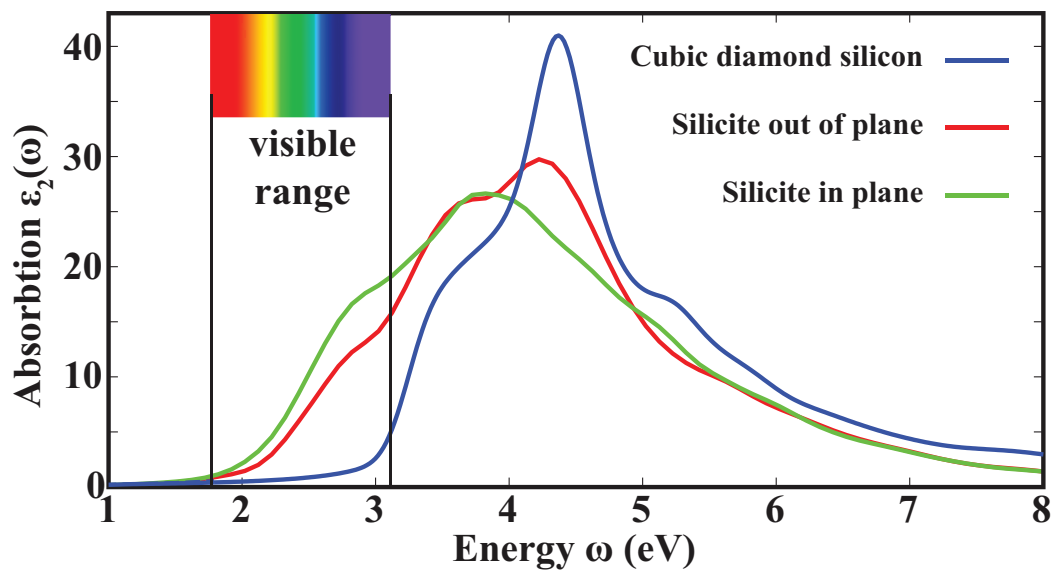


Figure 3: Absorption spectra for cubic diamond silicon and silicite. Silicite has significantly higher absorption in the visible range.