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Silicene on Silicide a Surface Science Approach to Materials Discovery¹

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Silicene like graphene is in its flat conformation a honeycomb structure with a Dirac cone at the K and K points of the Brillouin zone. In other respects, graphene and silicene are surprisingly different, which can be traced back to the relative stability of sp³ versus sp² type bonding and leads to a wide range of geometries defined by buckling z and conformation. The perfect sp² type layer would be planar, the high buckled configuration approaches the structure of the Si(111) surface. Control of buckling and conformation is critical to the future realization of exotic quantum materials which are predicted for silicene but have so far eluded experimental realization. Our recent study of MoSi₂ oxidation using scanning tunneling microscopy and spectroscopy (STM, STS) lead to the discovery of the silicene-terminated h-MoSi₂ (0001) surface, which is formed via a complex high-temperature $(\sqrt{3} \times \sqrt{3}) R30^0$ reconstruction. This reconstruction is geometrically identical to low buckled silicene and while it differs from the armchair configuration a Dirac type behavior is expected albeit not confirmed unambiguously. The silicene layer shows characteristic defect motifs and multiples of these defect motifs, where complete hexagons are removed from the silicene layer. Silicene layers with a Dirac-type electronic structure, can only be achieved if the perturbations, which stem from buckling, conformation and bonding to the substrate, are relatively small. In silicene buckling/conformation and substrate bonding are interdependent. I will discuss this interplay in the broader context and develop rules for substrate choice for silicene layers, and illustrate that the silicene-on-silicide platform is a particularly promising material combination. In addition, the feasibility of large area growth, which is required for future integration of silicene-on-silicide in device structures, and the study of its electronic structure, will be addressed.

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