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Substrate Effects on Silicene and How to Exploit Them

Udo Schwingenschlögl
King Abdullah University of Science and Technology (KAUST), Saudi Arabia

Silicene is the Si analogue of graphene with the same honeycomb structure and linear dispersions of the π and π* bands at the K point of the Brillouin zone. It is predicted to realize a buckled structure, due to sp^2-sp^3 hybridization, and is compatible with the current Si-based nano-electronics. Silicene yet has not been achieved by mechanical exfoliation but can be deposited on metallic substrates such as Ag (111), Ir (111), and ZrB_2 (0001). Regrettably, strong interaction to these substrates destroys the Dirac physics. For this reason, semiconducting substrates, including Si (111) and SiC (0001), have been explored theoretically to evaluate whether they lead to a Dirac cone with reasonable band gap (which is essential for applications). However, surface passivation is inevitable for these and similar substrates, due to their dangling bonds. Layered materials such as $MgBr_2$ (0001), MoX_2, and GaX_2 (X = S, Se, and Te), on the other hand, might preserve the characteristic electronic states of silicene and additionally simplify the preparation procedure as passivation is not required. The predicted effects of different substrates on silicene will be compared and evaluated with respect to technological requirements.

Biography:

Udo Schwingenschlögl is a Professor of Materials Science & Engineering at King Abdullah University of Science and Technology (KAUST). His research interests in condensed matter physics and first-principles materials modeling focus on two-dimensional materials, interface and defect physics, correlated materials, thermoelectric materials, metal-ion batteries, nanoparticles, and quantum transport.