

Abstract Submitted
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Physisorption of nucleobases on silicene and applications for DNA sequencing RODRIGO AMORIM, RALPH SCHEICHER, Uppsala University — We have used density functional theory including van der Waals corrections combined with the non-equilibrium Green's function (NEGF) method to study the adsorption of individual nucleobases on top of a 2-D allotrope of silicon, known as silicene, which was experimentally discovered to exist in a hexagonal buckled form. Our study focused on the stability, electronic properties and transverse electronic transport, i.e., changes in the transmission and the conductance caused by each base (A, C, G, T) in silicene compared to its pristine form. Intriguingly, despite the weak interaction between nucleobases and silicene, considerable changes in the transmittance at zero bias are predicted by us. This opens up the possibility to utilize silicene as an integrated-circuit biosensor as part of a lab-on-a-chip device.

Rodrigo Amorim
Uppsala University

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