New alternatives to improve biomolecules sensing using a 2D nanodevices

Rodrigo G Amorim and Ralph H. Scheicher

Division of Materials Theory, Department of Physics and Astronomy,
Uppsala University, Sweden

One of the challenges for the next generation of DNA sequencing is to have a robust, stable and feasible nanodevice. In this work we will show two different proposals along this direction. First, we will present one alternative as a device, hexagonal silicon 2D material, silicene. This material was recently discovered and has similar electronic structure compared to graphene but differs in its geometry (buckled structure) and the bonding (a combination of sp^2-sp^3 hybridization). In that case, as we can see in the top Figure, the nucleobases are adsorbed on the 2D material and it is extremely important to describe the interaction between the device (silicene) with the nucleobases (A, C, G and T). The standard DFT with GGA exchange correlation potential approximation is not capable to describe the long range interaction and take into account this type of interaction. We will show results for nucleobases on top of silicene employing an approximation with van der Waals correction and the transport calculation including this new computational ingredient. Intriguingly, despite the weak interaction between nucleobases and silicene, considerable changes in the transmittance at zero bias are predicted by us. Secondly, we will show how to improve the sensing of a graphene nanodevice to detect a single nucleobase. For this purpose we will use graphene with a nanogap with border functionalization (hydrogen or nitrogen). We used density functional theory (DFT) combined with the non-equilibrium Green's function (NEGF) method to study individual nucleobases in the graphene gap. We will show how to identify nucleobases with such a graphene nanogap devices (bottom Figure) and how we can improve the sensing of these devices.