Figure 1: A snapshot from the first-principles MD simulation of the oxidation process of silicene (Si; yellow, O; red, Ag; pink).

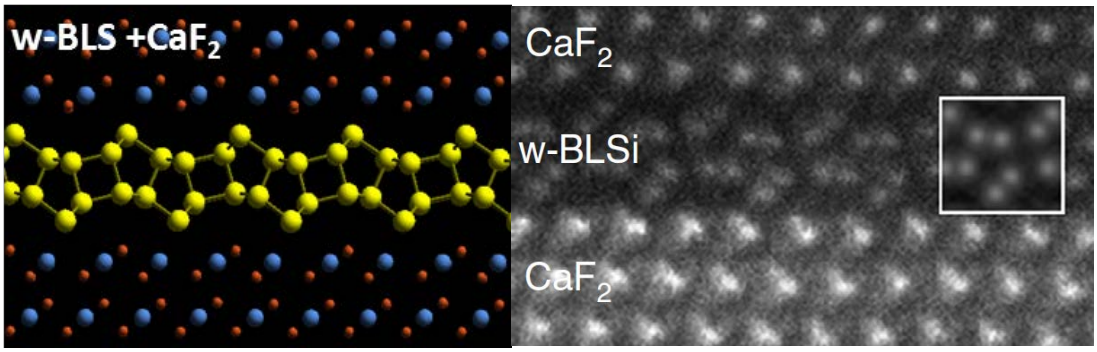

Figure 2: A bilayer silicene formed in a slit pore sandwiched by CaF_2 layers (left: theoretical prediction, right: experimental synthesis).

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General atomistic approach for modeling metal-semiconductor interfaces and surfaces

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Metal-semiconductor (M-SC) contacts play a pivotal role in a broad range of technologically relevant devices. Still, their characterization at the atomic-scale remains a delicate issue. One of the reasons is that the present understanding relies either on simplified analytical models often parametrized using experimental data [1], or on electronic structure simulations describing the interface using simple slab calculations [2]. Here we propose a general strategy to model realistic M-SC interfaces by using density functional theory (DFT) in combination with the non-equilibrium Green's function (NEGF) method as implemented in the Atomistix ToolKit (ATK) simulation software [3]. An accurate description of both sides of the interface is achieved by using a meta-GGA functional [4] optimally tuned to reproduce the SC measured band-gap, and a spatially dependent effective scheme to account for the presence of doping in the SC side. Compared to previous computational methods [2], the present approach has the important advantages of (i) treating the system using the appropriate boundary conditions and (ii) allowing for a direct comparison between theory and experiments by simulating the I-V characteristics of the interface. We apply this methodology to an Ag/Si interface relevant for solar cell applications, and test the reliability of traditional strategies [1,2] to describe its properties [5]. Finally, we will describe a novel surface Green's function (SGF) method where the surface is described as a true semi-infinite system and present a number of examples to

illustrate how the SGF method gives a number of benefits compared to the slab approach as well as enables new type of studies.

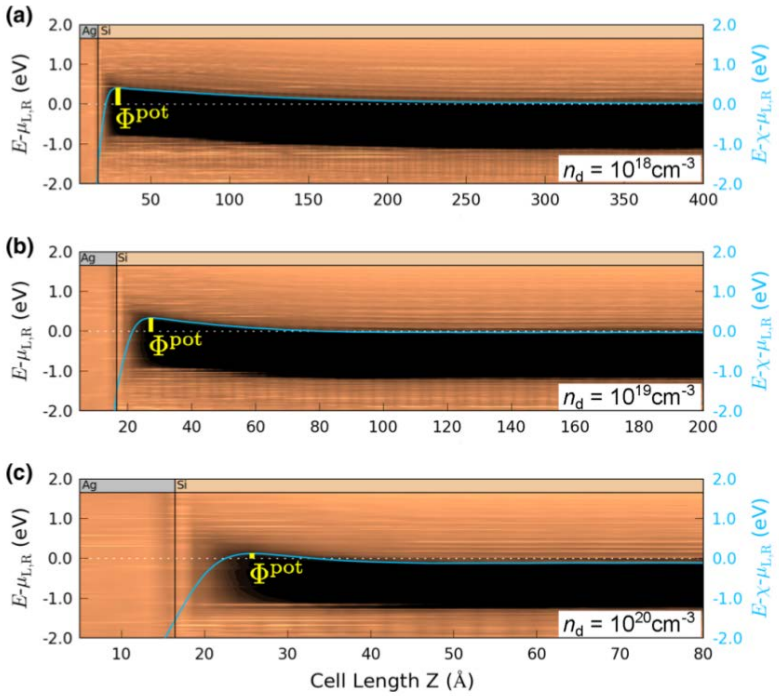

Figure 1. Local density of states (LDOS) of the two-probe setup at equilibrium for doping densities of 1018 cm^{-3} (a), 1019 cm^{-3} (b), and 1020 cm^{-3} (c). The energy on the vertical axis is relative to the system chemical potentials. Regions of low (high) LDOS are shown in dark (bright) color.

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