Design of advanced MoS_2/Si heterojunction photovoltaics.

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Among single junction photovoltaics, heterojunction solar cells based on crystalline silicon and amorphous silicon present the best efficiencies [1]. However, amorphous silicon can present high recombination rates, low conductivity and cause parasitic absorption [2].

We propose a model of photovoltaics cell in which the amorphous silicon is replaced by a thin layer of molybdenum disulfide MoS_2 [3]. MoS_2 is a two-dimensional material with a lamellar structure belonging to the class of transition metal dichalcogenides (TMD). Having the advantage of being naturally abundant and non-toxic, its lamellar structure also gives it interesting properties such as a tunable bandgap according to the thickness. Here we present the first steps towards the development of MoS_2/Si heterojunction photovoltaics that combine performance, non-toxicity and low costs, for applications in autonomous systems for the Internet-Of-Things

We perform numerical simulations with ATLAS Silvaco [4], in order to show the potential of such a structure, and to determine the optimal material parameters and the optimal design. We show that high quantum efficiencies and power conversion efficiencies of about 20 % can be attained.

In order to optimize the deposition of MoS_2, we perform optical and structural characterizations on thin layers of MoS_2 of different thicknesses, deposited on crystalline silicon (001), with silicon dioxide SiO_2 at the interface. The samples have the structure MoS_2/SiO_2 (80nm) /Si. Raman spectroscopy confirms the presence of multilayered MoS_2, while Atomic Force Microscopy (AFM) shows the presence of holes and outgrowths at the surface of the samples. X-ray Photoelectron Spectroscopy shows the presence of oxides in the layers of MoS_2, which explain the outgrowths and crackings seen in AFM. X-Ray Diffraction also confirms that, showing a change in the lattice parameters of MoS_2.

DFT simulations have just been started to figure out the effects of the presence of oxides on the MoS_2 parameters such as electron affinity, electron mobility, which may affect the performance of the photovoltaic devices.

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