Ab Initio Study of Octane Moiety Adsorption on H- and Cl-Functionalized Silicon Nanowires

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Silicon nanowires (SiNWs) are being intensively studied for both their peculiar properties and promising applications in a variety of field such as sensorics, photovoltaics, and micro-and optoelectronics. Due to their large surface-to-volume ratio, nanowires exhibit a superior sensitivity to chemical surface processes that allows to effectively tune the performance of nanomaterials. Surface functionalization is one of the best techniques to modify the electronic properties of SiNWs, which can also be controlled by exploiting the quantum confinement effects varying diameter and orientation of nanowire. For many specific device settings, the protection of the SiNWs surfaces against oxidation is a key issue. Therefore, it is necessary to predict and control the surface physical characteristics of oxide-free SiNWs, and to investigate the geometrical effects of organic molecule adsorption. To this end, first-principles calculations based on density functional theory (DTF), are a highly valuable tool to perform atomistic simulations very close to real nanotechnology experiments. We performed DTF calculations employing Quantum Espresso Ab-initio simulation package to investigate the electronic properties of different SiNWs oriented along the <112> direction. Modelling an octane moiety absorbed on the (111) and (110) surface of fully Cl- and H-functionalized SiNWs, we found that, while the diameter and the functionalization strongly affect the bandgap and the stability of the system, the Si-C bonds on the passivated surface can enhance protection against oxidation without substantial modification of the electronic properties.