AB-INITIO STUDIES OF THE SI(557)/AU AND SI(553)/AU RECONSTRUCTIONS

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Gold deposited on silicon surfaces at the monolayer regime results in a variety of reconstructions. The most interesting ones are the (quasi-) one dimensional phases, featuring monatomic wires of gold. They promise exotic physical phenomena, such as the Luttinger liquid [1]. These wires can be grown on the flat Si(111) surface which yields three possible directions for the wires to grow [2]. Stepped silicon surfaces avoid this problem; the wires grow parallel to the step edges. These systems have now been manufactured for years [3].

We present ab-initio studies of the Si(557)/Au and Si(553)/Au reconstructions using the Siesta ab-initio code [4].

The Si(557)/Au surface, resulting from the deposition of ~ 0.2 ML of gold, has been intensively studied, due to the rich physical phenomena observed in it. Our ab initio calculations show that spin-orbit coupling is crucial to understand the electronic structure of the Si(557)-Au surface [5]. The spin-orbit splitting originates the two one-dimensional bands observed in photoemission, which were previously attributed to spin-charge separation in a Luttinger liquid [6]. This spin splitting might have relevance for future device applications. We also show that the apparent Peierls-like transition observed in this surface by scanning tunneling microscopy is a result of the dynamical fluctuations of the step-edge structure, which are quenched as the temperature is decreased [7].

In the case of the Si(553)/Au reconstruction, we study a recently proposed model [3] and give some alternative models that yield bandstructures that are in good agreement with the photoemission data [8]. The role of the spin-orbit coupling is also studied.

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