# $\sqrt{7}\times\sqrt{3}$ Indium on Si(111): one or two indium layers?

**S. Rigamonti**[1], A. Arnau[1], T. Nagao[2] and D. Sánchez-Portal[1]

[1]Donostia International Physics Center (DIPC) and Centro-Mixto CSIC-UPV/EHU, San Sebastián, Spain
[2]National Institute for Materials Science, Tsukuba, Japan
santiago_rigamonti@ehu.es

Indium self-assembled overlayers on Si(111) are among the most studied metal-semiconductor surface nano-structures: A tremendously rich and complex structural phase diagram with more than 10 different overlayer reconstructions for up to two In monolayers (ML), as well as a wealth of structural and electronic phase transitions (e.g. the temperature driven $8\times2\Leftrightarrow4\times1$, the deposition driven $\sqrt{3}\times\sqrt{3}\Leftrightarrow2\times2\Leftrightarrow\sqrt{7}\times\sqrt{3}$, the field induced $\sqrt{3}\times\sqrt{3}\Leftrightarrow2\times2$)[1], have rised great interest in these surfaces.

At around one monolayer (ML) coverage, a commonly observed structure is the $\sqrt{7}\times\sqrt{3}$ reconstruction. This structure has been the subject of many experimental studies[2-5] that shed light on some fascinating structural and electronic properties, e.g., a Fermi surface strikingly close to the ideal two dimensional (2D) electron gas [4] or the recent discovery of superconductivity in this extreme 2D metal [5].

In spite of the accumulated experimental data, no general consensus has been reached to date on the number of In layers comprising the $\sqrt{7}\times\sqrt{3}$ nanostructure. Some experiments point to a single In overlayer model (SL), with In atoms arranged in a quasi-rectangular (-rec) or quasi-hexagonal (-hex) fashion with coverages of 1.2ML and 1.0ML respectively [2], while others support a double-layer (DL) model instead, with 2~3ML coverage [3]. Nonetheless, a precise determination of the overlayer structure at the atomic scale is the prerequisite for understanding its phenomenology.

In this contribution, we report ab-initio density functional theory (DFT) calculations for different In/Si(111) reconstructions (some of them shown in Fig. 1).[6] Our calculations were performed with the SIESTA code[7] within the local density approximation. We show that the Fermi surface (FS) and band-structure calculated for the SL-rec model of Kraft et al.[2] disagree with the experiments in Ref.[4]. We propose a DL structural model with 2.4ML coverage and find excelent agreement with experiments. For both the SL and the DL models the charge transfer from Si dangling bonds to the two dimensional gas is found to be negligible. We also show that the In-In interaction dominates over In-Si bonding.

## References


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## Figures

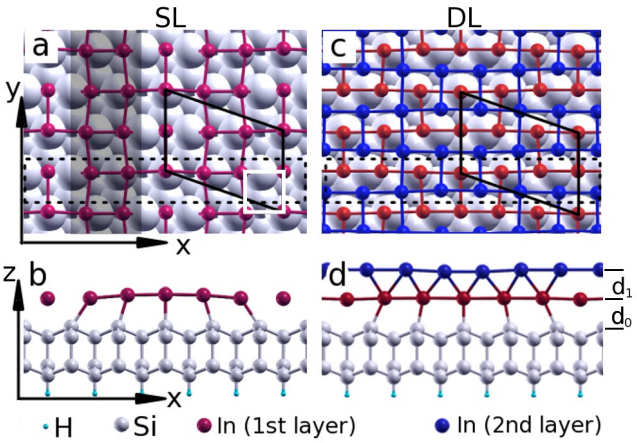


***Figure 1: Left**: SL-rec model. **Right**: DL-rec model. **a** and **c**: top views, **b** and **d**: side views of the structures.*