The Physics discipline in the School of Mathematical & Physical Sciences presents a seminar:

When: **Tuesday, 26th August, 2008, 1:00-2:00 pm**

Where: **P105 Physics Building**

The influence of C-defects at the Si(001) surface on In adsorption

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Abstract:
Recent scanning tunnelling microscopy and spectroscopy (STM/STS) observations show that the C-defects, which are commonly observed on the Si(001) surface, act as nucleation centres for In atoms diffusing on this substrate [1]. These measurements indicate that the Indium (In) atoms deposited on Si(001) tend to form chains of In dimers pinned to the defects. These experimental results strongly suggest that the presence of the C-defects increases considerably the local chemical reactivity of the silicon substrate. In this talk the results of our theoretical study related to this problem, based on the ab-initio density functional theory (DFT) calculations, will be presented and discussed. The aim of this study is to determine the mechanism responsible for the strong reactivity of the C-defects and the formation of the one-dimensional structures in the front of the defects by the diffusing adatoms. The obtained theoretical results will be analysed in the context of the existing STM/STS data.

P. Kocan et al. Phys.Rev. B**74** (2006) 037401