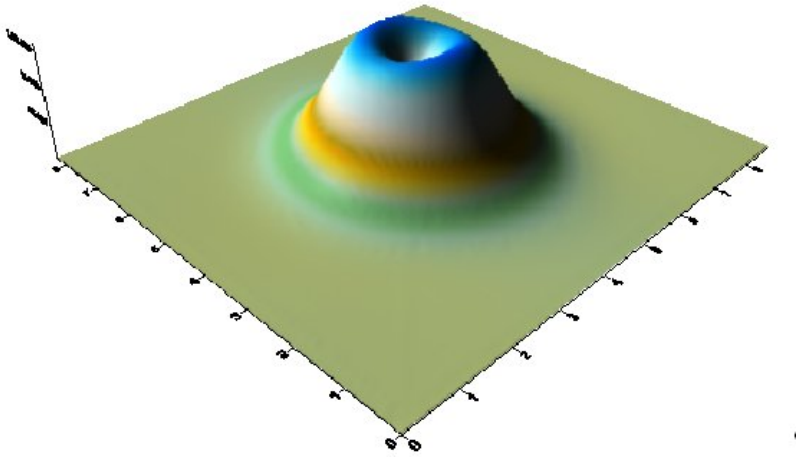
STSM Visit Report for Andres Arnau

INELASTIC TUNNELLING (REPORT)

During the three weeks I have been to Liverpool at the Surface Science Research Centre the advances in the project INELASTIC TUNNELING have been quite substantial. The first results of the collaboration with Dr. W.A. Hofer can be summarised as follows:

1. We have done first principle calculations of the electronic structure of Ag(110) surfaces with CO and C2H2 adsorbates. In the figure we show a three dimensional plot of the local density of states at 0.3 nm from the top most atom of CO/Ag(110). A clear inverted "sombrero" shape is seen, similar to the experimental findings [Phys. Rev. Lett. 87, 196102 (2001)].



2. We have also calculated the electronic structure of STM functionalised tips. The structure of the tips consists of a layered structure of W(110) planes with a CO or C2H2 molecule at the apex.

3. We have also calculated the vibrational modes of the adsorbed molecules on the surface.

The next step in the development of the project consists in the evaluation of the inelastic tunnelling current in Bardeen's approximation using both the tip and sample electronic structures. Presently, we are developing the computer code to do it. For a given vibrational mode of the adsorbate we calculate the perturbed sample wave functions that are needed to evaluate the overlaps. Once the overlaps are calculated the inelastic current can be calculated.