TIP EFFECTS IN IETS WITH THE STM

G. Teobaldi,[1] M. Peñalba,[2] A. Arnau,[3] W. Hofer[1] and N. Lorente[4]

[1]Surface Science Research Centre, University of Liverpool, L69 3BX, UK

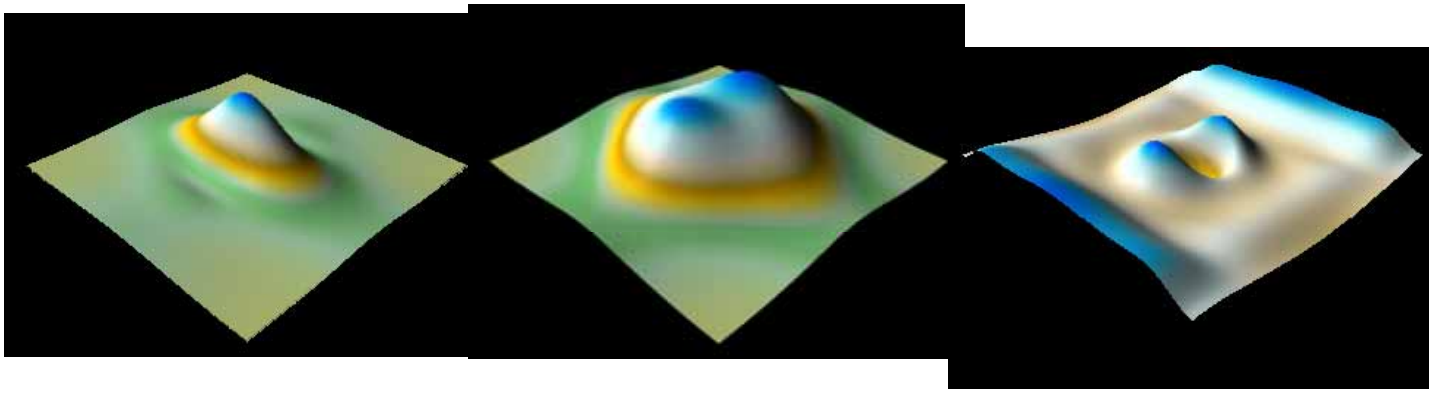
[2]Departamento de Física Aplicada, Escuela Universitaria Politécnica UPV/EHU, San Sebastián, Spain

[3]Departamento de Física de Materiales UPV/EHU, Facultad de Química, Unidad de Física de Materiales, Centro Mixto C.S.I.C-UPV/EHU, and Donostia International Physics Center (DIPC) San Sebastián, Spain

[4] Laboratoire Collisions, Agrégats, Réactivité, UMR 5589, IRSAMC, Université Paul Sabatier, 118 Route de Narbonne, 31062 Toulouse cedex, France

We have extended Bardeen's formalism as implemented in the code bSKAN[1] to include inelastic effects. These latter are produced by the coupling of tunnelling electrons and vibrational modes of a molecule adsorbed on a surface under the tip of the STM. The formalism follows the one of Ref.[2]. We have applied the new code to the vibrations of a CO molecule on different surfaces of Cu to calculate the elastic and inelastic contributions to the change in conductance due to the opening of inelastic channels. The inelastic efficiency (η) is defined as the ratio of the change in conductance due to the opening of the inelastic channel by the elastic conductance. In the figure we show the corresponding constant current maps η (x,y) for the frustrated rotation of CO on Cu(100) using a 4x4 surface unit cell and three different W-tips:

Sharp **Blunt** **CO-apex**



We find that:

(i) the frustrated rotation of the CO molecule is the mode that gives the strongest change in tunnelling conductance (around 10%),

(ii) the inelastic signal, as well as its spatial distribution, depend on the type of STM tip: from blunt metallic tips to sharp ones, and to molecularly functionalised ones.

[1] K. Palotas, W. A. Hofer, J. Phys.: Condens. Matter 17 (2005) 2705

[2] N. Lorente, Appl. Physics A 78 (2004) 799