

## **Ab-initio SP-STM of Co adatoms on the Au(100) and Au(111) surfaces**

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Among many fascinating phenomena, the scanning tunneling microscope (STM) has been used to detect the Kondo interactions between conduction electrons and single atomic spins and to study the properties of individual magnetic islands. Recently, inelastic electron tunneling spectroscopy (IETS) with an STM was used to measure the spin excitation spectra of individual magnetic atoms. Additionally, the STM can be used to manipulate and assemble individual nanostructures. Such atomic manipulation in situ was used to construct magnetic dimers and trimers, which displayed evidence of coupled-spin behavior.

In order to study these phenomena, we have used the projected augmented wave potentials method into the density functional theory (DFT) and coupled with the Tersoff-Hamman approach for STM imaging simulation of linear and triangular arrays of atomic-scale magnetic structures (Co adatoms on the Au(100) and (111) surfaces) for to study their electronic and magnetic structure. Depending of the Au surface, we have found strong interaction of the Co adatoms and different magnetic arrays. We present SP-STM imaging and spectroscopies of these different systems, at different tip magnetizations among other results.

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