DIRECTION DES SCIENCES DE LA MATIERE,
INSTITUT RAYONNEMENT MATIÈRE DE SACLAY

SERVICE DE PHYSIQUE ET DE CHIMIE DES SURFACES ET DES INTERFACES

SEMINAIRE *

Vendredi 28 mai 2010 à 11h00

Bâtiment 466, salle 111 - CEA Saclay, 91191, Gif sur Yvette

Magnetism at nanoscale: *ab-initio* density functional study and beyond

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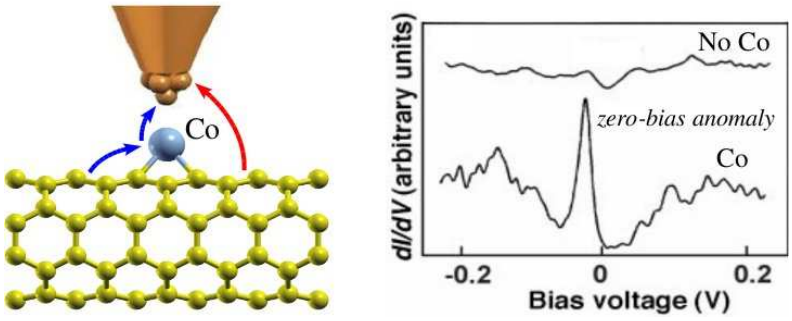
I will speak about our recent first principles studies on magnetism and electron transport in different nanosystems, mainly concentrating on two examples: i) bimetallic Ni/Au/Ni nanojunctions and ii) single magnetic impurities (Ni, Co, or Fe atoms) on Au nanowires and carbon nanotubes. The first system represents a classical set-up for studying magnetoresistance (MR) where the standard density functional theory (DFT) is expected to work well. We are especially interested here in the dependence of MR on dimensionality of the junction - from 2D planar interfaces to 1D nanowires and nanocontacts. The second system, on the contrary, represents a classical set-up for the Kondo problem, where a single magnetic impurity is coupled to a nonmagnetic conductor.
The many-body effects are expected to play here an important role, screening the impurity magnetic moment at low temperatures and modifying significantly the electrical conductance. We study these phenomena combining our DFT approach with the subsequent Numerical Renormalization Group solution of appropriate Anderson model.
All our DFT calculations were carried out with a plane wave package {\tt Quantum-ESPRESSO} (www.quantum-espresso.org). I will therefore discuss it in a more detail and will also say few words about other electronic structure codes available around.

Kondo in carbon nanotubes:



*** SERA PRECEDE D'UNE PAUSE-CAFE A PARTIR DE 10H30**

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