SACLAY

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DEPARTEMENT DE RECHERCHE SUR L'ETAT CONDENSE,
LES ATOMES ET LES MOLECULES,

SERVICE DE PHYSIQUE ET DE CHIMIE DES SURFACES ET DES INTERFACES

SEMINAIRE

Jeudi 30 Novembre 2006 à 14h00

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

Magnetic phenomena and electron transport in monatomic nanowires and nanocontacts

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Invité par M.C. Desjonquères

Abstract:

Metallic nanocontacts as thin as one atom can be now fabricated by means of two well-known techniques: scanning tunneling microscopy and mechanically controllable break junctions [1]. Due to the small size of such contacts, usually well below both the mean free path and the phase breaking length, the conductance even at room temperature is essentially ballistic and is simply proportional to the quantum-mechanical electron transmission at the Fermi energy. The latter is determined by the number of available transmission channels through the contact atom which is related to its valency.

I will first present some experimental results on the ballistic conductance of atomic-scale nanocontacts of different metals. It will be shown that in some metals (such as Au and Pt) the monatomic wires (atomic chains) can be formed before the breaking occurs. I will then give a brief overview of some theoretical methods for calculating the electron transmission function through atomic-scale conductors and will discuss in more detail our first-principles scattering approach [2]. Its main ingredients are the plane-wave basis set and ultrasoft pseudo-potentials and it has been recently extended to account for spin-orbit coupling [3]. The method is applied to study electronic, magnetic and transport properties of short monatomic Ni [4] and Pt [5] nanowires suspended between two semi-infinite leads. In the case of Pt, we find that spin-orbit effects are very important and modify significantly magnetic properties of the nanowire. For example, the free-standing monatomic Pt wire becomes magnetic even at the equilibrium interatomic distance. Moreover, the number of conducting channels (electron bands crossing the Fermi level) is considerably influenced by both spin-orbit interactions and by the presence of magnetism. The further interplay between the magnetism and the ballistic transport is investigated on example of three- and five-atom Pt nanowire in contact with two semi-infinite leads.

[1] N. Agrait, Phys. Rep. 377, 81 (2003).
[2] H.J. Choi and J. Ihm, PRB 59, 2267 (1999); A. Smogunov, A. Dal Corso, and E. Tosatti, PRB 70, 045417 (2004).
[3] A. Dal Corso, A. Smogunov, and E. Tosatti, Phys. Rev. B 74, 045429 (2006).
[4] A. Smogunov, A. Dal Corso, and E. Tosatti, Phys. Rev. B 73, 075418 (2006).
[5] A. Smogunov, A. Dal Corso, and E. Tosatti, in preparation.

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