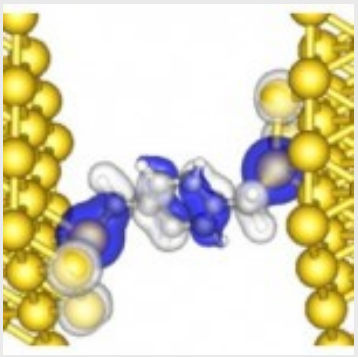
Calculating the Conductance of Single Molecule Junctions form First Principles



When: Friday, 11 September (2015), 12:00h
Place: Departamento de Física Teórica de la Materia Condensada, Facultad Ciencias, Module 5, Seminar Room (5th Floor).
Speaker: Héctor Vázquez, Center Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic.

Abstract:

In this talk I will present the group's recent work on single molecule transport. Our work uses DFT-NEGF methods to investigate the conducting properties of molecules placed between two metallic electrodes. I will first discuss the importance of linker chemistry and molecular chemical properties on elastic transmission. I will then briefly describe our recent efforts in mapping the different contributions to the inelastic vibrational signal.

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