Towards reality in modelling of molecular electronics (TRMME)

13.Jun - 17.Jun 2016

Cód. 132-16

Mod.:
Presencial

Edición
2016

Tipo de actividad
Workshop

Fecha
13.Jun - 17.Jun 2016

Ubicación
Palacio Miramar

Idiomas
Inglés

Web
http://trmme.dipc.org/

DIRECCIÓN

Daniel Sánchez Portal, CSIC-UPV/EHU

Comité Organizador

Descripción

As standard silicon technologies approach their fundamental limits, the exploration of molecular electronics, and other related bottom-up technologies, as viable alternatives is attracting an increasing amount of attention worldwide. Molecular electronics opens a wealth of opportunities related to the use of building blocks with built-in functionalities defined with atomic-scale precision by chemical means. However, it is also creates many difficult challenges related, for example, to the optimization of the device architectures and the control of interfaces between the device and electrodes and gates. Theory also faces important challenges to understand and simulate the properties of these new devices. Some of these challenges are fundamental, and related to the complex interplay between electron-electron correlations, electron-phonon interactions and interference in open quantum systems, pointing to the limitations of the current theoretical frameworks to correctly describe those phenomena. The complex and largely unknown (and difficult to control) structure of molecular junctions, and the links of the molecular blocks to the electrodes, also poses a fundamental problem for reliably predicting their properties. New theories and methodologies are being developed to overcome some of these limitations with the ultimate goal of optimizing the design and predicting the properties of molecular electronic devices. In this workshop we will bring together researchers actively working in different aspects of the of transport properties of atomic and molecular scale devices to advance towards this common goal. The focus will be on the theory, although there will be a few selected experimental talks, since our aim is to make connection with current experimental activity.

Objetivos

The aim of the TRMME workshop is to bring together experienced and young researchers, as well as students, working in the field of the theory of quantum transport and the development of computational tools for transport simulations in the nanoscale. The workshop aims to cover the following topics: • Large-scale calculations of quantum transport • Architectures: towards molecular-scale devices • Inelastic transport: vibrations and magnetic excitations • Multi-scale modeling of molecular electronics • Coupling of transport to light • Time dependences in molecular-scale transport • Effect of electron-electron interactions and correlations • Prediction of complex structures and growth

Website of the congress: http://trmme.dipc.org/

Colaboradores específicos del curso

Dirigido por:

Daniel Sánchez Portal

CSIC-UPV/EHU

Precios matrícula

REGISTRATION	HASTA 30-06-2016
INVITED SPEAKER	0 EUR
ATTENDANT	300,00 EUR

Lugar

Palacio Miramar

Pº de Miraconcha nº 48. Donostia / San Sebastián

Gipuzkoa