



# Towards reality in modelling of molecular electronics (TRMME)

**13.Jun - 17.Jun 2016**

**Cod. 132-16**

**Mod.:**

Face-to-face

**Edition**

2016

**Activity type**

Workshop

**Date**

13.Jun - 17.Jun 2016

**Location**

Miramar Palace

**Languages**

English

**Organising Committee**

Fundación  
BBVA



## Description

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 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.

## Course specific contributors



## Directed by



**Daniel Sánchez Portal**

CSIC-UPV/EHU

---

# Registration fees

<b>REGISTRATION</b>	<b>UNTIL 30-06-2016</b>
INVITED SPEAKER	0 EUR
ATTENDANT	300,00 EUR

# **Place**

## **Miramar Palace**

Gipuzkoa