

Theoretical Methods in Molecular Spintronics (TMspin)



17.Sep - 20.Sep 2018

Cod. Z07-18

Mod.: Face-to-face

Edition 2018

Activity type Workshop

Date 17.Sep - 20.Sep 2018

Location Materials Physics Center (CSIC-UPV/EHU)

Languages English

Academic Validity 40 hours

Organising Committee









Description

Magnetic molecules and atoms studied by scanning probe microscope experiments and molecular transistors represent ideal systems to address the very foundations of the quantum theory of magnetism. The proposed workshop will gather both physicists and chemists to question what electronic structure theory to use for such systems. Hence, the most recent developments in *ab-initio* methods will be presented with a special focus on those that could describe correlation effects, excitations and complex structural details on equal footing.

Organizing committee:

Andrea Droghetti, Universidad del País Vasco, Donostia-San Sebastian (chair)

Ivan Rungger, National Physical Laboratory, Teddington, UK

Tim Wehling, University of Bremen, Bremen, Germany

Objectives

The workshop aims at advancing electronic structure theory in order to accurately describe.

Magnetic properties of molecules in the gas phase, in particular spin state energetics and exchange coupling between several magnetic centres.

Magnetic properties of atoms and molecules on surfaces, in particular the Kondo effect and the surface mediated exchange-coupling between adsorbed atoms.

Finite-bias transport and magnetic excitations at the atomic scale.

Description of entangled states from first principle and application to quantum computation in magnetic molecules and atoms.

Course specific contributors





Directed by



Andrea Droghetti

Registration fees

REGISTRATION FEES	UNTIL 20-09-2018
INVITED SPEAKER / ORGANIZER	0 EUR
REGULAR FEE	

Place

Materials Physics Center (CSIC-UPV/EHU)

Manuel de Lardizabal, 4. 20018 Donostia / San Sebastián

Gipuzkoa