

Aim: the High performance computing for next generation nanomaterials & nanodevices engineering workshop is an event, to be held at the Catalan Institute of Nanoscience and Nanotechnology (ICN2), sponsored by the RED ESPAÑOLA DE SUPERCOMPUTACION-RES (<https://www.res.es/>), and which aims at presenting the use of high performance computing (HPC) in forefront research in nanomaterials, molecular electronics and nanodevices, to potential users of the RES HPC resources. The event will count on the presence of European experts in the field of nanoscience and nanotechnology, with strong focus on HPC applications, as well as representatives from the RES.

Workshop coordinators

José Hugo Garcia Aguilar
Stephan Roche
Marc Vila

Catalan Institute of Nanoscience and Nanotechnology (ICN2)

Registration

The registration is **free** of charges but participants should apply. Participant willing to present a poster should notify it in their applications.

Due to space limitations, maximum number of participant is 40.

To the selected participant the event will provide with: Conference material, 1 lunch and 3 coffee breaks.

To register send a motivation letter and simplified CV to josehugo.garcia@icn2.cat before **March 1, 2018**.

Keynote Speakers

Yann-Michel Niquet
CEA, INAC L_Sim, Université Grenoble FRANCE

Presentation Title

Leveraging on HPC for the modelling of nanoscale silicon devices in microelectronics.

Xavier Blase
Institut Néel-CNRS, FRANCE

Embedded many-body perturbation theory for organic and hybrid systems.

Carme Rovira
Universitat de Barcelona & ICREA, SPAIN

Computational simulation of biological processes.

Elisa Molinari
University of Modena and Reggio Emilia, ITALIA

Materials design at the Exascale.

Invited Speakers

Presentation Title

Stephan Mohr
Barcelona Supercomputing Center, SPAIN

The importance of High Performance Computing to accelerate Material Discovery

Juan Ignacio Beltran
Complutense University of Madrid, SPAIN

Oxygen vacancy stabilization of quantum-well energy levels in a ferroelectric-domain-wall tunnel junction.

Fernando Martin
Departamento de Química,
Universidad Autónoma de Madrid, SPAIN

Attosecond electron and nuclear dynamics in molecules.

Annapaola Migiani
Institut de Química Computacional i Catàlisis,
Universitat de Girona, SPAIN

Theoretical Excited-State Perspective on Heterogeneous Photocatalysis:
Water and Methanol Oxidation on TiO₂.

Marta Renato
Barcelona Supercomputing Center, SPAIN

The Spanish Supercomputing Network: resources and access

Tutorials

Tutorial title

Zheyong Fan
Aalto University, FINLAND

High-performance molecular dynamics simulations with GPUMD.

José H Garcia
Catalan Institute of Nanoscience and Nanotechnology,
SPAIN

Scalable iterative methods for non-equilibrium quantum transport
in gigascale systems.