

ICN2 is a renowned research centre. Its research lines focus on the newly discovered physical and chemical properties that arise from the behaviour of matter at the nanoscale.

The Institute promotes collaboration among scientists from diverse backgrounds (physics, chemistry, biology, and engineering) to develop basic and applied research, while seeking out new ways to interact with local and global industry.

It also offers researchers training in nanotechnology, develops numerous activities to promote and enable the uptake of nanotechnology by industry, and promotes networking among scientists, engineers, technicians, business people, society, and policy makers.

ICN2 was accredited in 2014 as a Severo Ochoa Centre of Excellence and is a founding member of the Barcelona Institute of Science and Technology (BIST). The aim of the Severo Ochoa Program, sponsored by the Spanish Ministry of Economy, Industry and Competitiveness, are to identify and support those Spanish research centres that demonstrate scientific leadership and impact at global level.

**Job Title:** Modelling two-dimensional-based gas sensors

**Research area or group:** Theoretical and Computational Nanoscience Group

**Description of Group/Project:** The host develops cutting-edge theoretical research on quantum transport phenomena in graphene and 2D materials and has a long experience in large-scale simulations of complex materials. In-house methodologies allow the simulation of disordered materials containing up to hundred millions atoms, enabling predictive modelling and collaboration with experimental and technology research. The group has been funded by company such as SAMSUNG, and is member of the Graphene Flagship project since 2014.

The project is connected to an EU-FET project in which European industries and engineering laboratories will develop novel generation of gas sensors, while the group will be in charge of the modelling tasks to guide the experimental towards optimisation of devices and support the interpretation of measurements.

**Main Tasks and responsibilities:**

The candidate will conduct numerical simulations of the optical and electrical conductivity of graphene under CO<sub>2</sub> or water adsorption. These simulations will assess the impact of unwanted surface contamination on the electrical output signals. Calculation of the variations of electrical and thermal conductivities of a “heated graphene patch” will be performed using molecular dynamics and time-evolution Kubo transport methods to deduce a relative change with respect to the reference situation (absence of CO<sub>2</sub> or water). Comparison with experimental data will be achieved to extract the intrinsic signals from parasitic ones and access the upper sensitivity limit of the detector structures.

**Education, Experience, Knowledge and Competences required:**

Theoretical physics and quantum simulations (molecular dynamics DFT and/or tight-binding modelling), and experience in device simulation or simulation of photodetectors would be a plus. Fluent in English.

## **Research Career Profile (According to the European Framework for Research Careers):**

R3 - Established Researcher

### **Summary of conditions:**

- Full time work (37,5h/week)
- Contract Length: 4 years
- Salary will depend on qualifications and demonstrated experience.
- Salary according to the cost of living in Barcelona.
- Support to the relocation issues.
- Life Insurance.

Estimated Incorporation date: December 2018

### **How to apply:**

All applications must be made via the ICN2 website <http://jobs.icn2.cat/job-openings/146/modelling-two-dimensional-based-gas-sensors> and include the following:

1. A cover letter.
2. A full CV including contact details.
3. 2 Reference letters or referee contacts.

Deadline for applications: November 1, 2018

### **Equal opportunities:**

ICN2 is an equal opportunity employer committed to diversity and inclusion of people with disabilities.