The mission of the Catalan Institute of Nanoscience and Nanotechnology (ICN2) is to achieve the highest level of scientific and technological excellence in Nanoscience and Nanotechnology. Its research lines focus on the newly-discovered physical and chemical properties that arise from the behavior of matter at the nanoscale. ICN2 has been awarded with the Severo Ochoa Center of Excellence distinction for two consecutive periods (2014-2018 and 2018-2022). ICN2 comprises 18 Research Groups, 7 Technical Development and Support Units and Facilities, and 2 Research Platforms, covering different areas of nanoscience and nanotechnology.

Job Title: Senior SIESTA Developer

Research area or group: Theory and Simulation

Description of Group/Project:
The Theory and Simulation Group developes efficient methods for atomistic simulations in nanostructured systems, which can fully exploit modern computer multiprocessor architectures, and applies them to selected problems in Nanoscience and Nanotechnology. These include (but are not restricted to) the SIESTA (see www.icmab.es/siesta) and TranSIESTA codes. SIESTA is a multi-purpose first-principles method and program, based on Density Functional Theory, which can be used to describe the atomic and electronic properties of systems with up to several thousands of atoms. SIESTA's versatility and efficiency have placed it in a position of relevance in a number of research areas, and its involvement in high-profile international projects (e.g. the EU MaX Center of Excellence) and other initiatives (e.g. CECAM's Electronic Structure Library (ESL)) have significantly expanded the scope and complexity of the software development effort.

Main Tasks and responsibilities:

• Play a leading role in the coordination and steering of the software development work in the Siesta ecosystem.
• Maintain fluid communication with the expanding network of Siesta developers and contributors, to handle coding plans and merge requests.
• Maintain high standards of documentation, testing, and deployment.
• Interface to the international initiatives in which Siesta is actively involved (the MaX EU Center of Excellence, the Electronic Structure Library, etc.)
• Follow best practices for continuous improvement of the development tools and workflow.
• Understand the relevance to the project of new developments in the wider fields of electronic-structure simulation methods and high-performance computing.
• Collaborate with the ICN2's IT personnel for the management of the group's scientific computing hardware and software infrastructure.
• Contribution to other activities in the group.

Education, Experience, Knowledge and Competences required:

• PhD-level training in computational materials physics/chemistry with ab-initio methods.
• At least two years of experience in post-doctoral research in the field.
• Past significant involvement in the development of a first-principles electronic-structure simulation code. Working knowledge of the internals of Siesta would be ideal.

• Strong coding skills. Proficiency in Fortran programming is a must, as is advanced knowledge of MPI-based parallelization techniques.
• Expertise in the handling of modern software engineering tools: version control and development platforms, build and deployment systems, documentation methods.
• Ability to communicate efficiently in fluent spoken and written English and to manage multiple threads of interaction.
• Initiative to keep abreast of key developments in the field.
• Strong motivation to advance the state of the art in materials simulation.

Summary of conditions:

- Full time work (37,5h/week)
- Contract Length: Permanent
- Salary will depend on qualifications and demonstrated experience.
- Support to the relocation issues.
- Life Insurance.

Estimated Incorporation date: as soon as possible

How to apply:
All applications must be made via the ICN2 website https://jobs.icn2.cat/job-openings/231/senior-siesta-developer and include the following:

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

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