The Nanoscience Cooperative Research Center, CIC nanoGUNE, located in Donostia / San Sebastian, Basque Country (Spain), is currently looking for a

SOFTWARE ENGINEER

to work on

Machine Learning for Materials Design

NanoGUNE is a research center devoted to conducting world-class nanoscience research for a competitive growth of the Basque Country. NanoGUNE is a member of the Basque Research and Technology Alliance (BRTA) and is recognized by the Spanish Research Agency as a María de Maeztu Unit of Excellence.

The Theory Group led by Prof. Emilio Artacho is looking for a software engineer candidate who will work on the development of state-of-the-art Machine Learning (ML) techniques applied to Materials Design. The **candidate** will be responsible for implementing, evaluating and testing modern quantum and classical ML techniques to predict novel materials for hydrogen storage, alternative ways of hydrogen production for internal combustion engines and fuel cells. Access to a quantum computer will be provided.

Key Responsibilities include:

- Gather training data from materials databases and their generation with active learning.
- Process the data to make it accessible to the ML models.
- Find suitable descriptors to feature the molecular and chemical systems.
- Select and train different ML models/architectures (Quantum and Classical ML).
- Evaluate and compare the performance of the models.
- Write product documentation, demos, and training material.

Required Knowledge/Skills/Abilities:

- Minimum 1 year of professional software development experience.
- Bachelors or coursework in Computer Science, Applied Mathematics, Physics, or related fields.
- Fluent in Python and C++.
- Comfortable working in Linux and macOS.
- Experienced in Unit Testing.
- Versed Git user.
- Good spoken and written English.

- Comfortable working in an international team.

We offer an international and competitive environment promoting teamwork in a diverse and inclusive environment. We welcome all applicants regardless of age, disability, gender, nationality, race, religion, or sexual orientation.

The **position** is expected to start on 01/01/2023 and go on for up to 2 years in the Theory group. https://www.nanogune.eu/en/research/groups/theory.

Candidates should **apply** by completing the form below and attaching the following documents:

1. A complete CV, motivation letter, certificates and 2 reference contacts, all grouped in a single PDF file

The **deadline** for applications is **31/12/2022**.

NOTES:

(i) All applicants will receive an answer after the end of the selection process; but please note that due to the large number of submissions that are expected, we cannot provide individual feedback.

(ii) Additional information about nanoGUNE's commitment towards HR excellence in Research and Gender Equality are available on our website.

(iii) We encourage you to subscribe to our HR mailing list to receive information related to nanoGUNE's open positions and open calls for different training and talent attraction programs.