



DC 5	Lead-free anti/ferroelectrics optimized for energy storage
Host Institution	Luxembourg Institute of Science and Technology
Supervisor	Jorge Íñiguez-González
Duration	36 months
Subject Area	Atomistic materials simulations, machine-learning methods, ferroelectrics, energy storage
Doctoral degree	Doctoral Programme in Physics and Materials Science, University of Luxembourg

Description

Supercapacitors with high energy storage density are nowadays in high demand to power IOT sensors. Recently, there has been increasing interest in purely electrostatic solid-state supercapacitors based on highly polarizable materials, e.g., ferroelectrics and antiferroelectrics. This project will focus on identifying strategies to optimize the energy-storage performance of ZrO₂-based anti/ferroelectric materials. The selected candidate will investigate the physical mechanisms controlling intrinsic materials performance, which will be studied by explicit quantum mechanical simulations based on density functional theory calculations, as well as by suitable machine-learned force fields which will enable larger-scale calculations. The candidate will spend a period of time at the IBM-research headquarters in Zurich, at the University of Groningen and at the University of Minho to interact with the experimental groups fabricating the energy storage capacitors.

Project-specific selection criteria:

- Master's degree (or equivalent) in physics, materials science or related discipline.
- Excellent Computational Physics/Numerical Simulation skills and background.

Other criteria:

- Good written and verbal communication, including presentation skills.
- Proficient English language skills.
- Good organisational skills, attention to detail and the ability to meet deadlines.
- Ability to think logically, create solutions and make informed decisions.
- Willingness to work collaboratively in a dynamic research environment.
- A strong commitment to his/her own continuous professional development.
- Willingness to travel and work across Europe.

Additional information

As part of the MSCA programme, all recruited MASAUTO researchers must comply with the Horizon Europe MSCA eligibility criteria:

- Doctoral Candidates must not have a doctoral degree at the date of the recruitment by the host organisation.
- At the time of recruitment by the host organisation, DCs must not have resided or carried out their main activity (work, studies, etc.) in the country of their host organisation for more than 12 months in the three years immediately prior to the recruitment date. Compulsory national service and/or short stays such as holidays and time spent as part of a procedure for obtaining refugee status under the Geneva Convention are not taken into account.

