

Company Description

CIC Energigune is a Cooperative Research Centre founded in 2007 with its headquarters in the Basque Country. Created thanks to the investments of the Basque Government and several leading companies in the energy sector, it aspires to become a true international leader in the field of energy and contribute to the industrial competitiveness of Basque companies.

Information

 Deadline: 2019-09-21
 Category: Business
 Province: Alava

 Country: Basque Country

Company

CIC energigUNE



Main functions, requisites & benefits

Main functions

CIC energigUNE (CICe) offers the opportunity to complete a PhD in the field of Computational Modelling at the Atomic Scale of Electrolyte Dynamics in Metal-air Batteries. The offer is aimed at motivated students who have good academic records and are ready to carry out a challenging and exciting 3-year applied research project. Who are we? CIC energigUNE is an excellence research center based in the Basque Country (Spain) and dedicated to the research and development of materials for energy storage. It offers the opportunity to work in an interdisciplinary and international environment. It is committed to affirmative action, equal opportunity and the diversity of its workforce. CICe is well equipped with a wide range of up-to-date facilities that are fully available for all its researchers. It also has a strong commitment in the long-term high-level training of its young researchers, and as proof of its training capacities, it indeed participates in numerous formative activities of national and international students through several programs at undergraduate, Master and PhD levels. Since 2011, CICe has been training more than 30 PhD students.

Requisites

We are searching for a highly motivated and independent researcher with a Master degree in Physics, Chemistry, Materials Science or other related topics. Students who expect to obtain their Master degree before September 2019 can also apply.

Good knowledge in quantum mechanics and statistical mechanics is expected and interest in writing computer code (e.g., Python) and shell scripts is an asset.

Experience with interatomic potentials for molecular dynamics simulations is desirable, but not essential

Experience with density functional theory methods, such as electronic structure calculations using VASP, Quantum Espresso, FHI-aims and/or similar packages is an advantage.

Basic experience with machine learning algorithms and/or network science is an advantage.

The candidate should also be able to work independently and as part of a highly ambitious research team, as well as have very good command of English.

He/she should be a good team player who can collaborate with other scientists. Highly motivated person and interested in investigation. She/he will be incorporated to a multidisciplinary team.

Benefits

The project involves the development and application of density functional theory calculations and Reax FF-based molecular dynamics simulations, which will enhance our atomistic understanding of non-aqueous liquid electrolytes of interest for next-generation battery technologies. The simulations will focus on ionic transport, electrolyte-electrode interactions, and aging mechanisms for different chemistries in metal-air battery systems. The project will be carried out in close collaboration with other CIC-