



## Postdoc in Computational High-Throughput Screening of Ion Conductors

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CIC energigUNE is a renowned energy research center, with headquarters in the Basque Country (Alava, Spain), which aims to be a benchmark in the field of energy storage.

The Atomistic Modelling and Computational Simulations group at CIC energigUNE is searching for a Postdoctoral researcher to be involved in an Industrial project.

### Job function:

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- Screening fast ion conductors by combining nano informatics with quantum-mechanical and bond valence method simulations.

### Qualification requirements:

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- We are searching for a highly motivated and independent researcher with a PhD in Physics, Chemistry, Materials Science or other related topics.
- The candidate shall possess a strong background (at least two years of previous experience as demonstrated, for instance, by first author publications) in Solid-State Physics/Chemistry and Quantum Chemistry, in particular, molecular quantum mechanics, statistical mechanics, and molecular simulation methods applied to bulk inorganic solids or polymers.
- Good expertise in density functional theory electronic structure calculations with extensive experience with codes such as VASP, FHI-aims, or CASTEP is required.
- Experience with machine learning algorithms and/or network science is strongly preferred. And experience in writing computer code (e.g., Python) and shell scripts is an asset.
- The candidate should also be able to work independently and as part of a team, as well as have very good English skills.
- Therefore, the successful candidate must be able to effectively communicate with a variety of audiences.

### **What we offer:**

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We are offering an **18-month** contract and advantageous professional development opportunities within interesting Industrial project with the possibility of renewal based upon satisfactory job performance, continuing availability of funds, and ongoing operational needs.

The candidate will join a multidisciplinary and collaborative team of theorists and experimentalists from condensed matter, materials, and chemical sciences.

**The position must start in November 2019.**

### **How to apply:**

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All applicants are invited to submit detailed curriculum vitae, contact information of at least three references and a cover letter detailing specific experience and scientific interests at [www.cicenergigune.com](http://www.cicenergigune.com).

**The selection process ends once a candidate is selected.**

CIC energigUNE is committed to affirmative action, equal opportunity and the diversity of its workforce.