## Job Offer

**Topics:**

The Basque Center for Applied Mathematics - BCAM, is looking for a **Research Technician position in Atomistic Simulations of Composite Electrolyte Materials embedding high entropy oxide particles** to join Modelling and Simulation in Life and Materials Sciences (MSLMS) group, and work under the supervision of Drs. Elena Akhmatskaya, Mauricio Rincón Bonilla, and Henry Andrés Cortés.

We are offering a unique opportunity for a motivated individual to join the Basque Center for Applied Mathematics (BCAM) as a Research Technician. This position involves working in collaboration with Prof. E. Marinero from Purdue University (USA) and Prof. Javier Carrasco from CIC energYGUNE (Basque Country, Spain), we will investigate CPEs containing lithium-doped high entropy oxide (HEO) fillers of the type \((\text{Mg,Co,Ni,Cu,Zn})_{1-x}\text{Li}_x\text{O}\), which have been reported to display a "colossal" dielectric constant and may help screening the polymer / Li-ion interactions, thereby enhancing Li-ion mobility (Berardan et al. Status Solidi RRL 10 (2016) 328–333 (2016); Liu et al. Chem Asian J. (2022), e202200839). Moreover, XRD analysis suggests that oxygen vacancies in the HEO preferentially locate at the particles surface, acting as potential anion trapping sites and thus increasing the Li-transference number (i.e., the ratio of Li-ion/anion diffusivity).

While experimental results are promising, a fundamental description of the mechanisms at play is lacking. By using a simplified HEO model, we will examine how the distribution of vacancies in the particle and the resulting dielectric constant impact the Li-ion and anion dynamics in the CPE. In addition, we aim to determine the mechanisms leading to the "colossal dielectric constant" of these particles and establish schemes to modulate this important parameter.

We will exploit our recent framework, originally developed to investigate CPEs comprising polyethylene oxide – LiTFSI matrix embedding conductive Ga-doped LLZO filler particles.
(Cortes et al. Macromolecules 56 (2023), 4256-4266; Bonilla et al. J. Colloid Interface Sci. 623 (2022), 870-882; Bonilla et al. ACS Appl. Mater. Interfaces 13 (2021), 30653-30667). Such framework will be extended to mesoscopic systems by introducing coarse-grained descriptions of the polymer and anion molecules.

The initial contract duration will be of 4 months with ample possibilities for extension, if the evaluation is positive. Our hope is to later on incorporate the research technician within BCAM's doctoral programme, subject to satisfactory performance.

If you are a young graduate passionate about Computational Physics, Chemistry, Applied Mathematics, Computer Science, or related fields, and eager to embark on a research career at BCAM, this opportunity is for you. Apply now and become part of our dedicated team at BCAM.

| Pls in charge: | Elena Akhmatskaya  
| Mauricio Rincón Bonilla  
| Henry Andrés Cortés |

| Salary and conditions: | The gross annual salary of the position will be 19.764€-29.994€ |
| It will then be on your own responsibility to make your yearly income declaration at the Bizkaia Treasury Agency. |
| Additionally, we offer a moving allowance up to 1.000€. Should the researcher have a family at the time of recruitment: |
| 1. 1.000€ gross in a single payment will be offered (you must be married-official register or with children and the certificate to prove it must be sent). |
| 2. 600€ gross per year/per child (up to 2 children) will be offered (the certificate to prove it must be sent). |

Free access to the Public Health System in Spain is provided to all employees.

| Nº Positions offered: | 1 |
**Contract and offer:** 4 months contract with possible extension

**Deadline:** August 15th, 2024, 14:00 CET (UTC+1)

**How to apply:** Applications must be submitted on-line at: [https://joboffers.bcamath.org](https://joboffers.bcamath.org)

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### Scientific Profile Requested

**Requirements:**
- Applicants must have their Bachelor’s or (preferably) Master’s degree in Computational Physics, Chemistry, Applied Mathematics, Computer Science, or related fields.

**Skills and track-record:**
- Although the requirements can be adapted to the different candidate profiles, a strong candidate needs to possess the following skills:
  - Good interpersonal skills.
  - Demonstrated ability to work independently and as part of a collaborative research team.
  - Ability to present and publish research outcomes in spoken (talks) and written (papers) form.
  - Ability to effectively communicate and present research ideas to researchers and stakeholders with different backgrounds.
  - Fluency in spoken and written English

**Scientific Profile:**
- The preferred candidate will have:
  - Basic background in atomistic simulation methods such as Molecular Dynamics (atomistic, coarse-grained) and Monte Carlo.
  - Basic knowledge of GROMACS and/or LAMMPS and atomistic visualization software (VMD, Ovito).
  - Working knowledge of Linux and job schedulers (e.g. Slurm, Torque, etc).
  - Basic knowledge in materials science and electrochemistry (desirable).

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### Application and Selection Process

**Formal Requirements:**
- The selected candidate must have applied before the application deadline online at the webpage: [https://joboffers.bcamath.org](https://joboffers.bcamath.org)
- The candidates that do not fulfil the mandatory requirements will not be evaluated with respect to their scientific profile.

**Application:**
- Required documents:
<table>
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<tr>
<th>Evaluation:</th>
<th>Based on the provided application documents of each candidate, the evaluation committee will evaluate qualitatively: the adaption of the previous training and career to the profile offered, the recommendation letters, the main results achieved (papers, proceedings, etc.), the statement of past and proposed future research and other merits; taking in account the alignment of these items to the topic offered.</th>
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</thead>
</table>

**Incorporation:** As soon as possible