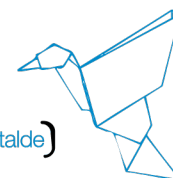


## Research Technician in Atomistic Simulations of Composite Electrolyte Materials

Job Offer	
Topics:	Atomistic Simulations of Composite Electrolyte Materials
PI in charge:	Elena Akhmatskaya Mauricio Rincón Bonilla
Salary and conditions:	<p><b>The gross annual salary of the Fellowship will be 18.000 - 26.000€.</b></p> <p>It will then be on your own responsibility to make your yearly income declaration at the Bizkaia Treasury Agency.</p> <p>There is a moving allowance for those researchers that come from a research institution outside the Basque Country from EUR 500 to EUR 1.000 gross.</p> <p><i>Free access to the Public Health System in Spain is provided to all employees.</i></p>
No Positions offered:	<b>#1</b>
Contract and offer:	<b>6 months contract</b>
Deadline:	<b>30 July 2021 at 14:00 CET (UTC+1)</b>
How to apply:	Applications must be submitted on-line at: <a href="http://www.bcamath.org/en/research/job">http://www.bcamath.org/en/research/job</a>

Scientific Profile Requested	
Requirements:	<ul style="list-style-type: none"> <li>• Promising young researchers.</li> <li>• Applicants must have their Bachelor's or Master degree preferable in Physics, Chemistry, Mathematics, Computer Science, or related fields.</li> </ul>
Skills and track-record:	<ul style="list-style-type: none"> <li>• Good interpersonal skills.</li> <li>• Demonstrated ability to work independently and as part of a collaborative research team.</li> <li>• Ability to present and publish research outcomes in spoken (talks) and written (papers) form.</li> <li>• Ability to effectively communicate and present research ideas to researchers and stakeholders with different backgrounds.</li> <li>• Fluency in spoken and written English.</li> </ul>

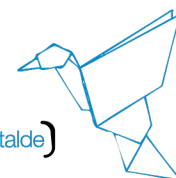


Scientific Profile:	<p>The preferred candidate will have:</p> <ul style="list-style-type: none"> <li>• Basic background in atomistic simulation methods such as Molecular Dynamics and/or Density Functional Theory.</li> <li>• Basic knowledge of GROMACS or/and LAMMPS and atomistic visualization software.</li> <li>• Working knowledge of Linux and job schedulers (e.g. Slurm, Torque, etc).</li> </ul> <p>Basic knowledge in materials science and electrochemistry (desirable).</p>
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Application and Selection Process	
Formal Requirements:	<p>The selected candidate must have applied before the application deadline online at the webpage <a href="http://www.bcamath.org/en/research/job">http://www.bcamath.org/en/research/job</a></p> <p>The candidates that do not fulfil the mandatory requirements will not be evaluated with respect to their scientific profile. Additional documents could be requested during the evaluation process so as to check this fulfilment.</p>
Application:	<p>Required documents:</p> <ul style="list-style-type: none"> <li>▪ CV</li> <li>▪ Letter of interest</li> <li>▪ 2 recommendation letters (desirable)</li> </ul>
Evaluation:	<p>Based on the provided application documents of each candidate, the evaluation committee will evaluate qualitatively: the adaption of the previous experience to the profile offered, previous projects managed, the letter of interest, and other merits; taking in account the alignment of these items to the job offered.</p>

<b>Incorporation:</b>	<b>As soon as possible.</b>
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<b>Research topic description:</b>	<p>Li-ion batteries have triggered a revolution in portable electronics that has considerably changed our lifestyle. However, the organic liquid electrolytes in use today are flammable and cannot be employed along with metallic lithium electrodes, which could significantly increase energy density. Solid-state electrolyte materials can reduce the risk of fire in case of battery failure and can, in principle, address the issues associated with replacing graphite electrodes by metallic lithium.</p> <p>In composite solid-state electrolytes (CSSEs), hard</p>
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	<p>ceramic particles (filler) are embedded within a flexible polymer matrix. The polymer provides mechanical flexibility and intimate interfacial contact with the electrodes, while the filler reinforces the polymer and reduces its crystallinity. Our aim is to provide a fundamental background for the rational design of this type of CSSEs.</p> <p>We have recently investigated polyethylene oxide (PEO) - LiTFSI complexes embedding conductive <math>Ga_xLi_{7-3x}La_3Zr_2O_{12}</math> (<math>Ga_x</math>-LLZO) filler particles, using a combination of in-house hybrid Monte Carlo methods and Molecular Dynamics simulations (ACS Appl. Mater. Interfaces, 2021). The next step is to examine the interface of (PEO) – LiTFSI/<math>Ga_x</math>-LLZO CSSEs at different Ga contents (<math>0.15 &lt; x &lt; 0.30</math>) for a range of conditions and settings. From the results, the researcher should conclude whether the LLZO particle composition has a significant impact on the structure and conductivity of the polymer phase. The study will be conducted in collaboration with CIC energyGUNE and Purdue University.</p>
<p><b>Keywords:</b></p>	<p>Solid-state Li-ion batteries, composite solid-state electrolytes, LLZO, PEO, Hybrid Monte Carlo simulations, Molecular Dynamics.</p>

