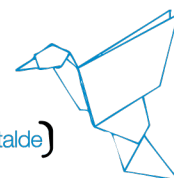


PhD in Modelling and in-silico Screening of Composite Electrolytes for Next-generation Lithium Batteries

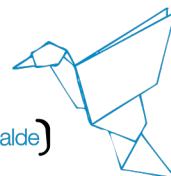
Job Offer	
Topics:	<p>The research activity will involve the development and application of density functional theory calculations, enhanced sampling molecular simulations, and utilisation of machine-learned interatomic potentials which will improve the atomistic understanding of composite electrolytes based on polymer matrices and inorganic fillers for solid-state batteries. The implementation of newly developed numerical techniques and computational models/approaches in the in-house software packages as well as in popular open-source software codes will be important part of this research. The simulations will focus on studying ionic transport through solid-solid interfaces. The results will then be disseminated in high-impact publications, conferences and open software codes.</p> <p>The research will be performed in Modelling and Simulation in Life and Materials Sciences group at BCAM and in Modelling and Computational Group at CIC energiGUNE.</p>
PI in charge:	Elena Akhmatkaya (BCAM) and Javier Carrasco (CIC energiGUNE)
Salary and conditions:	<p>The gross annual salary of the Fellowship will be 18.450 the first year, and the following years must be reviewed yearly based on Spanish EPIF legislation.</p> <p>Additionally, we offer a moving allowance up to 1.000€.</p> <p>Should the researcher have a family at the time of recruitment:</p> <ol style="list-style-type: none"> 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).



	<p>2. 600€ gross per year/per child (up to 2 children) will be offered (the certificate to prove it must be sent).</p> <p><i>Free access to the Public Health System in Spain is provided to all employees.</i></p>
Contract and offer:	3 years
Deadline:	March 10th, 2023 14:00 CET
How to apply:	Applications must be submitted on-line at: http://www.bcamath.org/en/research/job

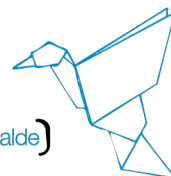
Scientific Profile Requested	
Requirements:	We are searching for a highly motivated and independent researcher with a Master degree in Physics, Chemistry, Materials Science or other related topics.
Skills and track-record:	The preferred candidate will possess good interpersonal skills, will demonstrate ability to present and publish research outcomes in spoken (talks) and written (papers) form. The candidate should be able to work independently and as part of two highly ambitious interdisciplinary research teams, as well as have very good command of English.
Scientific Profile:	The preferred candidate will have a good knowledge in quantum mechanics and statistical mechanics and be able to write computer codes in Python, C++ or Fortran and shell scripts. Experience with density functional theory methods, such as electronic structure calculations using VASP, Quantum Espresso, FHI-aims or similar packages is also required. Background in atomistic simulation methods such as Molecular Dynamics and/or Monte Carlo applied to solid state materials is highly desirable. Experience with interatomic potentials for molecular dynamics simulations and basic knowledge of machine learning methods and Bayesian analysis at user level would be desirable, but not essential.

Application and Selection Process	
Formal Requirements:	The selected candidate must have applied before the application deadline online at the webpage http://www.bcamath.org/en/research/job



	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.
Application:	Required documents: <ul style="list-style-type: none"> ▪ CV ▪ Letter of interest ▪ 2 recommendation letters ▪ Statement of past and proposed future research (2-3 pages)
Evaluation:	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.

Incorporation:	<i>Before 30th of June 2023</i>
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**IC2023_02 BCAM
International Call**

