basque center for applied mathematics

EXCELENCIA SEVERO OCHOA

IC2021_12 BCAM International Call

Research Technician for the Atomistic Simulation of Hydrogen Diffusion in alloys

Job Offer	
Topics:	Hydrogen diffusion, atomistic modelling, kinetic Monte Carlo, Molecular Dynamics, Density Functional Theory, metal alloys, Hydrogen diffusion, mesoscale models.
PI in charge:	Elena Akhmatskaya and Mauricio Rincon Bonilla
Salary and conditions:	**The gross salary of the Research Technician will be 18.000 - 26.000€.** It will then be on your own responsibility to make your yearly income declaration at the Bizkaia Treasury Agency. 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. *Free access to the Public Health System in Spain is provided to all employees.*
Contract and offer:	3 months (with possible extension, subject to performance review)
Deadline:	**December 15th 2021 14:00 CET**
How to apply:	Applications must be submitted on-line at: 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.

Scientific Profile Requested	
Requirements:	• Promising young researchers, prospective PhD students. Applicants must have their Bachelor's or Master degree preferable in Computational Physics, Computational Chemistry, Applied Mathematics, Computer Science, or related fields.
Skills and track-record:	• 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: • Strong background in atomistic simulation methods such as Molecular Dynamics and kinetic Monte Carlo applied to solid state materials. • Basic knowledge of LAMMPS and/or GROMACS and atomistic visualization software. • Working knowledge of Density Functional Theory. • Experience in hydrogen diffusion in alloys, embrittlement processes and/or crack propagation. • Background in mesoscopic simulation methods is desirable. • Programming skills in either Python, C++ or Fortran are desirable.

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: ▪ CV ▪ Letter of interest, succinctly describing past research experience ▪ 2 recommendation letters (desirable)
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.) and other merits; taking in account the alignment of these items to the topic offered.

Incorporation:	**As soon as possible.**

Research topic description:	This work will be focusing on the atomistic modelling of hydrogen adsorption and diffusion in metal alloys. Under certain conditions, the presence of hydrogen may lead to loss of ductility, strength and/or toughness in metals, a phenomenon called hydrogen-induced embrittlement (HIE). HIE can pose a risk to the sustainability of oil and gas structures, gearboxes and anchors of offshore wind turbines or steel architectural constructions. Although causing a serious threat for metal structures, HIE remains a complex process that is not completely understood because of the variety and complexity of mechanisms. Here, we will tackle this issue from an atomistic perspective. The research technician will employ existing force fields combined with kinetic Monte Carlo and/or Molecular Dynamics to simulate intra- and inter-crystalline hydrogen diffusion in metal alloys of interest for the wind turbine sector.