# Postdoctoral Fellowship in Atomistic Simulation of Hydrogen Embrittlement in Steels

## Job Offer

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| PI in charge:            | Elena Akhmatskaya and Mauricio Rincon Bonilla                           |

| Salary and conditions:   | The gross annual salary of the Fellowship will be 28.000 - 32.000€.     |
|                         | 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 up to EUR 2.000 gross. |
|                         | Free access to the Public Health System in Spain is provided to all employees. |
|                         | This project will be funded by Elkartek project ICME KK-2021/00022.     |

| Contract and offer:      | 1 year (with possible extension, subject to performance review)          |

| Deadline:               | November 15th 2021 at 14:00 CET (UTC+1)                                  |

| 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:            | • Young and experienced researchers are both welcome to apply.           |
|                         | • Applicants must have their PhD completed before the contract starts.   |
Skills and track-record:
- Good interpersonal skills.
- A proven track record in quality research, as evidenced by research publications in top scientific journals and conferences.
- 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.
- Working knowledge of Density Functional Theory.
- Experience in hydrogen diffusion in steels, embrittlement processes and/or crack propagation is highly desirable.
- Background in SPD or other mesoscopic particle simulation methods is desirable.
- Programming skills in either Python, C++ or Fortran are desirable.
- Familiarity with GROMACS/LAMMPS/VASP/Quantum ESPRESSO is highly 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
**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 is framed within the Basque government funded ICME project, in which six agents of the Basque Science, Technology and Innovation Network (including BCAM) are involved. The purpose of ICME is the development of a multi-scale modelling methodology to establish the link between chemical composition and manufacturing processes with the resulting microstructure and mechanical properties of metal alloys. In BCAM, we will be focusing on the atomistic modelling of Hydrogen-induced embrittlement (HE) of steels, which can significantly reduce the ductility and load-bearing capacity and cause cracking and catastrophic brittle failures at stresses below the yield stress.

It is well established that HE is connected to the fast diffusion of hydrogen atoms through the solid materials lattice, often by quantum mechanical tunnelling (even at room temperature) followed by interaction with crystal defects. Unfortunately, diffusion of hydrogen through crystal defects and its impact on the mechanical properties of the material are fundamentally less understood than hydrogen diffusion in perfect crystal lattices. The postdoctoral fellow will combine density functional theory with kinetic Monte Carlo and/or Molecular Dynamics to simulate hydrogen diffusion at defect-rich steel grain boundaries, with the aim of extracting kinetic and thermodynamic parameters that can be employed by our partners in continuous phase field models to understand the influence of defect concentration, temperature, and steel composition on HE at a microscopic scale.
In addition, the researcher will use particle dynamics methods to simulate mesoscopic phenomena such as crack propagation in steels under diverse HE conditions, incorporating the parameters derived from the atomistic scale models described above.