POSTDOCTORAL FELLOWSHIP IN ATOMISTIC SIMULATION OF STEELS IN HYDROGEN – RICH

Company Description

BCAM is the Research Center on Applied Mathematics created with the support of the Basque Government and the University of the Basque Country, which aims to strengthen the Basque science and technology system, by performing interdisciplinary research in the frontiers of mathematics, talented scientists' training and attraction, so the excellence of our results are recognized by the Society

Information

Deadline: 2022-09-30
Category: Business
Province: Bizkaia
Country: Basque Country
City: Bilbao

Company

BCAM

Main functions, requisites & benefits

Main functions

This work is framed within the Basque government funded Elkartek project M-KONTAK, in which several agents of the Basque Science, Technology and Innovation Network (including BCAM) are involved. The purpose of M-KONTAK is the development of a multi-scale modelling methodology to fundamentally understand the behavior of steels in hydrogen-rich environments. In BCAM, we will be focusing on the atomistic modelling of Hydrogen-induced embrittlement (HE), which can significantly reduce the ductility and load-bearing capacity and cause cracking and catastrophic brittle failures at stresses below the yield stress. The postdoctoral fellow will combine density functional theory with kinetic Monte Carlo and/or Molecular Dynamics to simulate hydrogen diffusion at 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 morphology, temperature, and composition on HE at a microscopic scale.

Requisites

M.Sc. or B.Sc. degree in Mathematics, Statistics, Computer Science and related disciplines. Good interpersonal skills. Demonstrated ability to work independently and as part of a collaborative research team. Ability to effectively communicate and present research ideas to researchers and stakeholders with different backgrounds. Fluency in spoken and written English. Solid programming skills in Julia. Candidates without specific knowledge of Julia but excellent skills in structurally similar languages such as Python, MATLAB, C++ or Ruby may be considered. Background in optimization methods. Specific knowledge in metaheuristic techniques such as simulated annealing of harmonic search is highly desirable. Experience with molecular dynamics codes (GROMACS, LAMMPS, etc.) is desirable.

Benefits

The gross annual salary of the Fellowship will be 18.450€-28.000€ Contract: 12 months (extensible) 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: 1.000€ 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). 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.