basque center for applied mathematics

IC2022_08 BCAM International Call

Postdoctoral Fellowship in Atomistic Simulation of Steels in Hydrogen – Rich Environments

Job Offer	
Topics:	Hydrogen embrittlement, atomistic modelling, kinetic Monte Carlo, Molecular Dynamics, Density Functional Theory, steels, Hydrogen diffusion, mesoscale models.
PI in charge:	Elena Akhmatskaya and Mauricio Rincón Bonilla
Salary and conditions:	**The gross annual salary of the Fellowship will be 28.000 - 34.000€ according to experience.** 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 2.000€. Should the researcher have a family at the time of recruitment: 1. 2.000€ 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). 2. 1.200€ 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.*
Contract and offer:	2 years (performance evaluation after first year)
Deadline:	**October 14th 2022 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 to check this fulfilment.

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Scientific Profile Requested	
Requirements:	• Young and experienced researchers in computational Physics, Chemistry, Materials Science, and related areas are 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 alloys, embrittlement processes and/or crack propagation is highly desirable. • Background in mesoscopic simulation methods is desirable. • Programming skills in Python, C++ or Fortran.

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 M-KONTAK project, 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.

EUSKO JAURLARITZA
GOBIERNO VASCO