

Research Technician on atomistic simulation of gas mixtures in membrane reactors

Job Offer

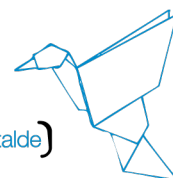
Offer

The Basque Center for Applied Mathematics is looking for a Research Technician (RT) to join the Modelling and Simulation in Life and Materials science group led by Prof. Elena Akhmatskaya in the atomistic simulation of carbon molecular sieve membranes (CMSMs) for the separation of water/methanol mixtures.

The results from this work will provide valuable insights for optimizing membrane performance in "e-methanol" production, a critical step in the European push for greener freight transport. This position will have an initial duration of 4 months. This project is funded by the Basque Government through the Elkartek Lurka grant, a transformative Initiative that aims to develop a renewable fuels hub in the Basque Country by combining classical-quantum simulation, experiments and AI. The RT will be directly supervised by Senior Fellows Dr. Mauricio Rincón Bonilla and Dr. Bikram Kumar Das.

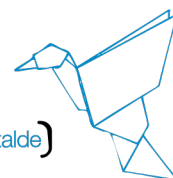
Electrofuels (e-fuels) are synthetic fuels produced by combining captured carbon dioxide with green hydrogen, offering a viable pathway to decarbonize heavy transport. Their production can be streamlined using membrane reactors, which are integrated devices that simultaneously combine chemical processing with gas separation. Within these systems, CMSMs (robust, nanoporous carbon materials that separate gas molecules based on precise differences in kinetic diameter) constitute highly effective separation barriers. Developing robust thermodynamic and mass transport models to predict permeation behavior under varying operational conditions, optimize membrane architecture, and reliably scale up the separation units required for large-scale synthetic fuel deployment.

As "e-methanol" emerges as a vital sustainable fuel for maritime shipping, optimizing its production via membrane reactors is increasingly critical. To advance this task, the RT will model the separation of water/methanol mixtures using carbon molecular sieve membranes (CMSMs) functionalized with surface oxygen



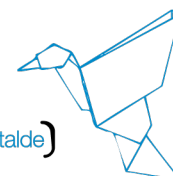
	groups. By coupling classical atomistic methods with coarse-grained interatomic potentials, the RT will simulate molecular adsorption and diffusion within the sub-nanometer pores of CMSMs. We will evaluate these dynamics as a function of surface hydrophilicity under typical operating conditions. Finally, by integrating these atomistic insights with structural data from real membranes, we will predict macroscopic performance to guide future membrane design.
PI in charge:	Mauricio Rincón Bonilla and Bikram Kumar Das.
Salary and conditions:	The gross annual salary of the PhD student will be: 20.663 € - 29.075 € according to experience. <i>It will be your responsibility to file your annual income tax return with the Bizkaia Treasure Agency.</i> Additionally, we offer a moving allowance of up to 500€. Should the researcher have a family at the time of recruitment: 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). 2. 600€ gross per year/per child (up to 2 children) will be offered (the certificate to prove it must be sent). <i>Free access to the Public Health System in Spain is provided to all employees.</i>
Nº Positions offered:	1
Duration of contract:	3 months
Deadline:	August 30, 2026, 14:00 CET (UTC+1)
How to apply:	Applications must be submitted online at: https://joboffers.bcamath.org

Scientific Profile Requested	



Mandatory requirements:	Applicants must have a bachelor's or master's degree in computational physics, Chemistry, Applied Mathematics, Computer Science, or related fields. PhD students searching for an internship would also be considered.
Scientific profile:	• Basic background in atomistic simulation methods such as Molecular Dynamics and Monte Carlo schemes. • Basic knowledge of GROMACS and/or LAMMPS and atomistic visualization software (VMD, Ovito). • Basic knowledge of membrane science (desirable).
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.

Application and Selection Process	
Formal requirements:	The selected candidate must apply before the deadline online at: https://joboffers.bcamath.org The candidates that do not fulfil the mandatory requirements will not be evaluated.
Application:	Required documents: ▪ CV and academic record ▪ Letter of interest, including research interests ▪ 2 recommendation letters
Evaluation:	Based on the documents provided by each candidate, the committee will qualitatively evaluate: • alignment of the training and career of the candidate to the position offered • recommendation letters • letter of interest



- other academic and scientific merits

Date of start: October 1st, 2026



This RT position is funded by the LurKa project (KK-2026/00055), financed by the Basque Government through the ELKARTEK Program for the support of collaborative research.

