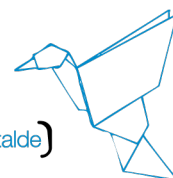


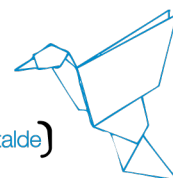
PhD student _MSCA-DN e-ChemIn (DC5): In-silico reconstruction of solid-liquid and solid-solid electrochemical interfaces at the nanoscale

Position description	
Reference:	Doctoral Candidate DC2
Title:	MSCA-DN e-ChemIn (DC5): In-silico reconstruction of solid-liquid and solid-solid electrochemical interfaces at the nanoscale
Hiring beneficiary:	Basque Center for Applied Mathematics (BCAM)
Location:	Bilbao, Spain
Research Field	Physics - Computational Physics Physics - Statistical Physics Chemistry - Molecular Chemistry Computer Science - 3D Modelling Computer Science - Modelling tools Computer Science - Programming Engineering – Materials engineering
Expected date of communication of results:	Less than 3 months after the application deadline.

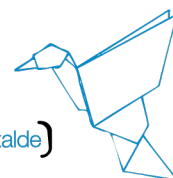
Job description	
Objective:	The aim of this project is developing inverse modelling and optimization techniques that leverage experimental data to construct detailed 3D representations of complex interfaces in energy storage and conversion devices at the atomistic level. These include solid-liquid (S-L) interfaces (e.g., between carbonaceous anodes and ionic liquid electrolytes in next-generation Na-ion batteries), and the solid-solid (S-S) interfaces (e.g., between metal oxide catalysts and carbon support materials to improve catalytic performance in water oxidation reactions). To achieve this goal, we will leverage BCAM's enhanced



	Bayesian sampling techniques, generalized hybrid Monte Carlo (MC) schemes, and adaptive integration methods designed to accelerate atomistic simulations. The approach to be developed will initially integrate spectroscopy data (XPS, SAX, SXRD) to generate candidate structures for S-S and S-L interfaces, which are subsequently refined using high-resolution microscopy (EELS, TEM) and NMR measurements. We will then deploy these refined, high-fidelity models to analyse the structural evolution of materials during electrochemical processes and to characterize interfacial ionic transport.
Expected results:	(1) A robust methodology for the in-silico reconstruction of complex materials implemented in an open-source code with a user-friendly interface. (2) Atomistic models free from standard idealization (e.g. defect-free, planar surfaces), with unprecedented detail of the interface chemistry, morphology. (3) A fundamental description of how typically overlook features, e.g. substrate heterogeneity and surface corrugation, shape interface performance in storage and conversion devices.
PhD enrolment	The selected candidate will be required to enroll in a PhD program at the University of the Basque Country (EHU) but will perform research activities at BCAM.
Supervisors:	Main supervisor: Prof. Elena Akhmatskaya (BCAM, https://www.bcamath.org/en/research/areas/m3a/mslms) Co-supervisor: Prof. Amaia Saracibar (EHU, https://www.ehu.eus/es/web/doktoregoa/doctorado-ciencia-tecnologia-materiales/profesorado?redirect=fichaPDI&idPdi=273081) Advisory support: Dr. M.R. Bonilla (BCAM, https://www.bcamath.org/en/research/areas/m3a/mslms) Co-supervisors from secondments: Prof. S. Dvinskikh (KTH, https://www.kth.se/profile/sergeid), Prof. J. Carrasco (CIC energiGUNE, https://cicenergigune.com/es/javier-carrasco-rodriguez)
Secondments (short term academic and industrial internships):	DC will stay 3 months at Leibniz Institute for New Materials (Prof. N. Tarakina) and 2 months at CIC energiGUNE (Prof. J. Carrasco), and 3 months at KTH Royal Institute of Technology (Prof. S. Dvinskikh).

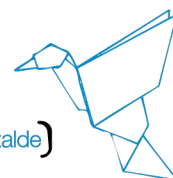


Vacancy requirements	
Qualifications:	Applicants must not already hold a doctoral degree at the date of recruitment and must not have resided or carried out their main activity (work, studies, etc.) in Spain for more than 12 months in the 36 months immediately before the recruitment date. Eligibility will be verified at the time of recruitment. Master's degree or equivalent in Applied Mathematics, Physics, Computational Chemistry or closely related disciplines.
Languages:	Excellent communication and writing skills, thorough command of the English language are mandatory.
Skills/Experience	• Experience with atomistic or particle simulations methods: Molecular Dynamics, Monte Carlo schemes, free energy methods. • Good knowledge of Bayesian inference, data science, and machine learning. • Experience in scientific computing in C++, Python, and/or Julia. • Knowledge of electrochemistry and materials science (desirable). • Ability to work as a member of an international, multi-disciplinary team.
Job details	
Salary:	The salary will comply with the rules of the 2025 MSCA Doctoral Network program under Horizon Europe and consists of: • a living allowance (country correction coefficient applies), • a mobility allowance (€710/month), • and, if applicable, a family allowance (€660/month). • Skilled workers who have not been fiscal residents in Spain for the last 5 years can enjoy a 30% tax exemption on their salary in Bizkaia for up to 10 years. All amounts are subject to national taxation and social security regulations.



Other benefits:	• Social Security coverage • Training, Networking and secondment opportunities • Career Development plan
Duration:	The position is funded for 36 months under the MSCA Doctoral Network. The total contract duration is 36 months.
Starting date:	From 01.11.2026 but not later than 01.04.2027
Type of contract:	Full-time employment contract in accordance with national regulations
Hours per week	Full time
Place of work:	The Basque Center for Applied Mathematics (BCAM) is located in Bilbao, Spain, and is an internationally leading centre for applied mathematics research, a scientific partner to national and international research institutions, and a provider of research and innovation for the regional and national industry. BCAM is an institute of the Basque Excellence Research Centres (BERC) network and has about 150 employees from over 10 nationalities. https://www.bcamath.org/en Alameda de Mazarredo 14 48009 Bilbao, Bizkaia (Basque Country, Spain)
Local language:	The knowledge of Spanish/Basque is a plus but not a requirement as English is a main working language at BCAM.

Application procedure and selection	
Applicants must submit:	• CV (including a detailed description of residence and main activities over the last 3 years). • Motivation letter. • Copies of academic degrees. • Contact details of 3 referees.
Deadline	20.09.2026



Apply via:	https://joboffers.bcamath.org/
Selection of candidates	Recruitment will follow the MSCA Doctoral Network principles of: • Open, transparent and merit-based selection • Equal opportunities and non-discrimination • Evaluation by a qualified selection committee Shortlisted candidates may be invited for interviews. The selection process will be properly documented in accordance with MSCA requirements.
Diversity Statement	BCAM promotes an open and inclusive institutional culture in which diversity is valued and actively fostered. As an equal opportunity employer, BCAM conducts this recruitment process in accordance with the HRS4R principles and the European Charter for Researchers, ensuring equal opportunities and non-discrimination. Candidate selection is based solely on scientific excellence, with active monitoring to promote gender balance and support underrepresented groups. The e-ChemIn project provides fair working conditions, comprehensive parental leave provisions, diversity training, and administrative and relocation support through EURAXESS channels.

