PhD candidate in the STEM characterization of twisted free-standing oxide films

The Institute of Materials Science of Barcelona (ICMAB-SCIC) is currently seeking a highly motivated candidate to sponsor the application of a doctoral **INPhINIT** fellowship from "La Caixa" Foundation to pursue PhD studies in our research center accredited with the Spanish Seal of Excellence "Severo Ochoa" (https://lacaixafoundation.org/en/doctoral-inphinit-fellowships-incoming-call). This candidacy is focus on STEM disciplines, with a maximum duration of 4 years, covering labor costs, research costs and doctoral tuition fees, plus on-site training program in multidisciplinary skills.

Description of the research project and group:

It has been recently observed that when two layers of a ferroelectric material are stacked with relative twist angles of several degrees, novel ferroelectric wave and vortex patterns form and they ascribe to the specific boundary conditions formed by the moiré pattern of the interface between membrane layers [*Nature* 626, 529–534 (2024)]. This simple strategy allows stabilizing intriguing ferroelectric patterns of electric polarization that could be leveraged for next-generation electronics. Here, we aim on the atomic scale investigation of emerging electric-polarization textures in 'twist-and-stack 'engineered free-standing layers of $BiFeO_3$ (BFO), a lead-free and room temperature multiferroic material with strong coupling between lattice (strain) and charge, spin and orbital parameters. The candidate will be devoted to the study of BFO heterojunctions stacked at different twist angles by plane-view and cross-sectional aberration-corrected scanning transmission electron microscopy (STEM) to characterize the atomic reconstructions at moiré points and study the local changes in lattice, electronic and vibrational (phonons) structures. The candidate will have access to cutting-edge microscopy platforms located at the ALBA synchrotron (Bellaterra, Barcelona), Institut Català de Nanociencia i Nanotecnologia (ICN2), the University of Barcelona (UB). The candidate will also have the opportunity to perform periodic research stays at the University of Chinese Academy of Sciences (UCAS, Beijing, China), one of the top laboratories for studies in ultra-high resolution electron energy loss spectroscopy (EELS).

The recruited PhD candidate will enroll the Materials Science PhD program at Autonomous University of Barcelona. The candidate will be supervised by Dr. Roger Guzman under the Nacional Project PID2023-149407NB-I00, and will join the Laboratory of Multifunctional Thin Films and Complex Structures (MULFOX) at the Institute of Materials Science of Barcelona (ICMAB-CSIC), one of the leading groups on the growth and characterization of complex oxides. As part of our team, the candidate will have the opportunity to collaborate with a large network of world leading researchers in the field of functional oxides in synergy with the use of advanced materials characterization, in particular with electron microscopy analytical methods.

Main tasks, responsibilities and benefits:

The focus of this project is on the atomic scale STEM characterization of novel ferroelectric polarization textures at the interface between two free-standing oxide films twisted with a relative angle. The main tasks that will be carried out within the project include:

- Use of focused ion beam (FIB) system to prepare samples for TEM/STEM investigations.
- Conventional-TEM characterization of moiré structures using dark-field electron diffraction imaging.
- Mapping of the emerging polarization textures and local electric fields using atomic-resolution STEM imaging techniques in combination with advanced four-dimensional (4D-STEM) characterizations to reveal the intricate polarization dependence with the local strain gradients and lattice deformation.
- Study local changes in the electronic structure at the moiré points evaluated by core-loss electron energy loss spectroscopy (EELS) and analysis of the fine structure.
- Study of the possible coupling of confined charges with vibrations of the lattice (phonons) using state-of-the-art monochromated vibrational EELS under the framework of our research collaboration with the University of Chinese Academy of Sciences (UCAS, Beijing, China).

AVAILABLE INSTRUMENTS

- Thermo Fisher Spectra 300 (60-300 keV), double corrected and monochromated, Gatan Continuum EELS with K3 direct electron detector, segmented and pixelated detectors, Super-X EDS system.
- Thermo Fisher Spectra ULTRA (30-300 keV), double corrected and monochromated, HR EELS, segmented and pixelated detectors, ULTRA-X EDS system.
- JEOL NEOARM (30-200kV), cold-FEG gun, probe corrected, Rio (CMOS) and Gatan K3 cameras, double EDXS detectors, segmented detector, multiple holders for in-situ experiments
- FEI F20 200 KeV STEM, EELS + EDX
- FIB Helios 5UX dual beam

Requirements of the call:

- BSc and/or MSc in STEM disciplines.
- Experience: candidates must not have carried out more than four years of research activity before the closing date of the call
- Studies pursued: at the time of recruitment, candidates must have completed the studies that allow them to enroll in an official PhD program in Spain/Portugal. The verification of the required level of studies will be carried out by the host university when the admission procedure begins.
- Candidates cannot have started doctoral studies prior to the start of the fellowship.
- Mobility:

  - *Incoming call:* candidates **must not have** resided or carried out their main activity (work, studies, etc.) in Spain/Portugal for more than twelve months in the three years immediately preceding the closing date of the call.
  - *Retaining call:* candidates **must have** resided or carried out their main activity (work, studies, etc.) in Spain/Portugal for more than twelve months in the three years immediately preceding the closing date of the call.
- Level of English: candidates must accredit the required level of English by submitting one of the certificates specified in the rules for participation.

What we offer:

- Participation in training events, group networks and dedicated workshops and schools for young researchers
- Participation in national and international workshops and conferences on the basis of the obtained results (E-MRS, MRS, ICACC, IMC…)
- Personal Career Development Plan (PCDP) during the first month of enrollment. The student will be enrolled at UAB Doctoral School "Materials Science Program" and we will promote a tailor-made training program offering compulsory and optional courses.
- Full time work (37,5 h /week)
- Contract length: Temporary, maximum of 4 years
- Salary: €35,800 per year to cover the fellow's labor costs (minimum annual gross salary of €25,000).
- €3,500 per year for research costs such as conferences, courses, research stays, consumables, equipment, charges for the use of intellectual property, etc.

Key dates:

1. End: 23 January 2025, at 2 pm Peninsular Spain
2. Shortlisting results and call for interviews: 11 April 2025
3. Selection interviews 28 and 29 May 2025
4. Final result: 6 June 2025

How to apply:

Applications have to be made through: https://fundacionlacaixa.org/ca/beques-doctorat-inphinit

Interested candidates can contact Dr. Roger Guzman for further information: rguzman@icmab.es

Why working with us:

ICMAB – CSIC is a multidisciplinary global reference center for the cutting-edge research of functional materials for electronics, energy and health which fosters knowledge transfer and it is characterized by its internationalization and its education, inclusion and diversity policies. ICMAB-CSIC is committed to know-how transfer to productive sectors as well as to participate

in educational and outreach activities. Since 2016, ICMAB -CSIC has been awarded for three consecutive periods with the Severo Ochoa Centre of Excellence distinction.

ICMAB-CSIC, with over 250 members from 47 nationalities, is a more than three decades old research institute located at the Universitat Autònoma de Barcelona (UAB) campus, surrounded by other research and technological centers and with access to many state-of-the art equipment and scientific facilities. Moreover, ICMAB-CSIC has its own scientific services equipped with the newest scientific instrumentation and with highly specialized technical staff available to the scientific community.

ICMAB-CSIC stands out for its great training activity at the doctoral level. Training on technical, scientific and transversal skills are offered to ICMAB-CSIC personnel. Moreover, ICMAB-CSIC has coordinated 2 Marie Sklodowska-Curie COFUND doctoral training programs on advanced functional materials: DOCFAM (2017-2022) and DOCFAM+ (2023-2028). In total, 48 doctoral students have been trained (18 at the at the ICMAB).