

Position Description

Group of research topics: Modelling and synthesis at the molecular scale

Position is funded by	<ul style="list-style-type: none"> - COFUND, Marie Skłodowska-Curie Actions (MSCA), Horizon 2020, European Union - Catalan Institute of Nanoscience and Nanotechnology (ICN2), Spain - RMIT University (RMIT), Australia
PhD awarding institution/s:	Dual PhD awarded by Autonomous University of Barcelona (UAB), Spain and RMIT
Locations	<ul style="list-style-type: none"> - Primary: Barcelona, Spain - Secondary: Melbourne, Australia - Annual workshops in Barcelona, Spain
Contract	Full time (36 months)
Gross annual salary	25.898 EUR (gross amount before employee's taxes and contributions)
Preferred start date	01/09/2022 (tentative)
Deadline for applications	30/04/2022 (Reference: ICN2-DC2)

Your choice of research topics (only one of these projects will be funded):

Project 1: Bridging time and length scales for the simulation of corrosion	Project 2: First Principles modelling of electrochemical processes	Project 3: Computational design of environmentally clean and non-toxic corrosion inhibitors
<p>Corrosion is a complex phenomenon, involving very different length and time scales, from atomistic to macroscopic. Computer simulations typically describe only a part of these scales. Multiscale approaches bring information back and forth between different scales, enabling a complete view of the overall process. The project will develop multiscale tools specifically designed to study corrosion in steel and aluminium alloys, of great importance for the transportation industry.</p> <p><i>Further information may be obtained from the Supervisors.</i></p>	<p>The project aims at developing methods to study electrochemistry at the atomic level, using first principles approaches like Density Functional Theory. The work will focus on being able to describe the interface between electrified surfaces and the liquid electrolyte, as a function of the applied voltage. The aim is to understand the chemical reactions taking place at the interface, with atomistic detail, and the electron transfer processes driving these reactions.</p> <p><i>Further information may be obtained from the Supervisors.</i></p>	<p>To protect metals from corrosion, avoiding cathodic and anodic reactions, chemicals are used as corrosion inhibitors that passivate the surface and delay the electrochemical processes. This project aims to design new environmentally-friendly inhibitors that replace the toxic industrial materials used today. This will be done using computer simulation tools and numerical methods, to gain insight into how molecular structure and functionality determine the response of inhibited coatings.</p> <p><i>Further information may be obtained from the Supervisors.</i></p>

Supervisors: <u>Prof. Pablo Ordejon (ICN2)</u> and <u>Ivan Cole (RMIT)</u>		
Research Fields: Corrosion; Density Functional Theory; Molecular Modelling; Multiscale Modelling	Research Fields: Corrosion; Density Functional Theory; Molecular Modelling; Multiscale Modelling	Research Fields: Corrosion; Density Functional Theory; Molecular Modelling; Multiscale Modelling

REDI

The REDI (RMIT European Doctoral Innovators) program is a unique opportunity offering excellent PhD conditions including enviable international experience, top-class research discipline and transversal skills training as well as networking with-academic and industry leaders across 60+ supporting partners and 12 countries.

As a REDI researcher you will be:

- enrolled by two entities, with the chance to be awarded dual doctorates and gain alumni status from multiple institutions, including the Marie Curie Alumni Association.
- seeing the world and spending a year at RMIT University in Melbourne, Australia (ranked in the top 20 of universities under 50 years old in the world).
- part of a rich multidisciplinary network of researchers and supervisors who come together in annual, week-long training events in Barcelona.
- working closely with industry and gaining experience with the 40+ leading companies supporting the program.
- earning a salary above national standards for doctoral positions with full social security benefits (with further support available for eligible researchers with additional needs).
- receiving support and guidance from two highest-calibre, experienced supervisors with high PhD completion rates.
- enhancing your career prospects through comprehensive technical and transversal skills training from leading institutions, intersectoral and international experience and mentoring.
- working on innovative and exciting projects of high commercial and societal value with up to four years to complete your research.

For more information visit: rediprogram.eu

Are you REDI? (Expected Profile)

Your background and skills: You should have a master's degree (Physics, Chemistry, Materials Science or Nanoscience will be preferred). You should also be educated and skilled in using classical molecular dynamics with some knowledge of DFT simulations. Good knowledge and skills in Quantum Mechanics is a must.

Your work experience: Work experience in using classical molecular dynamics, as well as some expertise on quantum mechanical simulations, either in the academia or the industry, will be highly valued.

Your research experience: Research experience on a research project within Master degree or beyond will be highly valued. Also, publications would be a plus.

Employment Benefits and Conditions

ICN2 offers a 36-months (extendable up to 48 months in duly justified cases) position based in Barcelona (Spain). International travel is foreseen to Australia (up to 12 months). There is a probation period of four (4) months and there are 37.5 working hours per week.

The remuneration, in line with the European Commission rules for Marie Skłodowska-Curie grant holders, will consist of a gross annual salary of est. 25.898,66 EUR gross per year (gross amount before employee's taxes and contributions). Of this amount, the estimated net salary* to be perceived by the Researcher is est. 1.700 EUR per month. However, the definite amount to be received by the Researcher is subject to national tax legislation. For more information on the estimated net monthly salary, please use the [net salary calculator](#).



**Net salaries can fluctuate in accordance with an individual's personal circumstances (marital status, age, disability, family and dependents, etc. The above indicative net salaries offer an approximation of what a single person in their early 20s could expect to receive in their bank account after taxes.*

Benefits include:

- Medical care under the Spanish public healthcare system and workplace accident insurance
- Support Relocation agency
- ICN2 social benefits: life insurance, flexible timetable, flexible compensation package.
- Training programme
- 1,000€ yearly travel allowance to cover flights and accommodation to participate in the annual workshop at RMIT Europe in Barcelona (Spain)
- 10,000€ allowance to cover flights and living expenses for up to 12 months in Australia

For more details, please see: <https://icn2.cat/en/careers/phd-programme/advice-to-candidates>

REDI to apply? First a little more about us...

ICN2

ICN2 is a flagship institute established to pursue excellence in the fields of nanoscience and nanotechnology. Its core activities include basic and applied research across a range of disciplines, incl. nanoelectronics, nanophotonics, nanophonics and nanofabrication, as well in technology transfer and public outreach. The centre comprises 18 research groups plus a highly specialised technical support infrastructure and hosts 280+ researchers from over 30 countries. It further includes within its mission to train students and early-career researchers, as well as create opportunities between researchers, industry, policy makers and society. ICN2 was recognised as a leading national Severo Ochoa Centre of Excellence in 2014, renewed in 2018. It is a founding member of the Barcelona Institute of Science and Technology (BIST) and is a member of the CERCA network of research centres of the Generalitat Catalunya. ICN2 has participated in 28 MSCAs, 12 of which are ongoing.

ICN2 offers to its Researchers a wide range of training, mentoring and support activities, including:

- **Mentoring programmes**
- **Courses and training opportunities:** languages trainings, health and safety, job related skills, organizational and personal skills and scientific knowledge.
- **Language courses:** ICN2 includes English, Spanish and Catalan language courses in the training plan every year.
- **Relocation support:** ICN2 provides support such as finding accommodation and assistance with bureaucracy (for residence work permit and VISA).
- **Cultural and social activities:** ICN2 has a social activity section on the intranet. It also offers welcome information on the first day and organizes an ICN2 Day with activities for all ICN2 Community.
- **Engagement with industry:** Strong interaction through the whole project will take place with the company SIMUNE, which is a SME based in San Sebastian (Spain) and focused on providing materials simulation services and software to industrial clients. The methodological advances made in the project will likely be further developed into commercial products in a joint R&D activity between ICN2, RMIT and SIMUNE, and further commercialised by SIMUNE, giving rise to authorship and economic rights among the participants in the development. Research stages at SIMUNE will be frequent.

For more information, visit: <https://icn2.cat/en/>

RMIT

RMIT is a global university of technology, design and enterprise, ranked in the top 20 of universities under 50 years old in the world. World-class people, leading edge resources, collaboration with industry partners and multi-disciplinary approaches are just a few of the trademarks of research at RMIT, which boasts almost 90,000 students and campuses in Australia, Vietnam, a centre in Barcelona, Spain and research and industry partners on every continent.



As Doctoral Student at RMIT you will be able to benefit from a wide range of training and mentoring opportunities including:

- **The PhD Up** program offering a huge range of workshops, seminars and short courses to build research knowledge and skills, including research writing, publishing, research methods, ethics, project management and careers (see more at: <https://www.rmit.edu.au/students/student-essentials/information-for/research-candidates/enriching-your-candidature/phd-up-program>)
- **RMIT PhD Online Modules**, designed specifically for PhD students, including *Researching your literature review*, *Writing a research proposal*, *Choosing where to publish*, *Writing for Publication*, *Research Integrity*, etc.
- **RMIT Creds**, RMIT's Digital Credentials Platform, which includes over 80 credentials covering a wide range of topics such as *Understanding Responsible Research and Innovation*, *Academic Integrity Awareness*, *Emotional Intelligence*, *Diversity Matters*, *Agile Ways of Working*, *Why Gender Matters*, *Cross Cultural Communications*, etc. (see more at: <https://www.rmit.edu.au/study-with-us/levels-of-study/short-courses>);
- **The e-Grad School**, the online learning modules of the Australian Technology Network (ATN) of Universities' covering a multitude of transferrable skills such as *Critical and Creative Thinking*, *Leadership and Communication*, *Entrepreneurship*, *Research Commercialisation*, *Public Policy*, etc.
- **The RMIT Mentoring platform also** gives you access to mentoring from trained professionals and experts, including:
 - o *Career Mentoring* - career guidance from industry professionals from all disciplines and global locations.
 - o *Women@RMIT Mentoring* - career guidance from industry professionals who are committed to gender diversity and equality in the workplace (especially for female students in male dominated industries)
 - o *Pride Mentoring* - a chance for students who identify as LGBTIQ+ to receive professional and social guidance from industry professionals who also identify as LGBTIQ+ or are familiar with the additional challenges these groups face in the workforce.

Find out more: rmit.edu.au

UAB

The Autonomous University of Barcelona is a leading university providing quality teaching in a wide variety of courses that meet the needs of society and are adapted to the new models of the Europe of Knowledge. Our courses provide students with outstanding practical experience, helping them to be better prepared as they enter the professional world. UAB is internationally renowned for its quality and innovation in research.

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In recent years, the UAB has seen recognition for its efforts in promoting quality in teaching, in attracting international talent and in obtaining a growing impact in research, together with a progressive improvement in its classifications in the most prestigious and influential international rankings. Thus, the UAB is well as occupying an outstanding position among Spanish universities in world rankings such as the QS World University Rankings (QS WUR), the Times Higher Education World University Rankings (THE WUR) and the Academic Ranking of World Universities (ARWU).

Find out more: <https://www.uab.cat/web/universitat-autonoma-de-barcelona-1345467954774.html>

A little more about you...

Eligibility

You need to fulfil criteria of the REDI program and both universities to be recruited.

To apply for REDI, you must comply with the MSCA-COFUND eligibility criteria by the application deadline:



- **Be in the first four years Full-Time Equivalent (FTE) research experience** of your research career and not yet have been awarded a doctoral degree. FTE Research Experience is measured from the date when a researcher obtained the degree entitling him/her to embark on a doctorate, **AND**
- **Not have resided or carried out your main activity (work, studies, etc.)** in the country of your research host for more than 12 months in the 3 years immediately before this call's deadline. Time spent as part of a procedure for obtaining refugee status under the Geneva Convention (1951 Refugee Convention and 1967 Protocol), compulsory national service and/or short stays such as holidays is not taken into account.

AND the following criteria:

- **Hold a bachelor's degree requiring at least 4 years of full-time study** in a relevant discipline awarded with honours and including a research component; **OR**
- **Hold a master's degree that includes a research component** or a master degree without a research component with at least a high distinction average; **OR**
- **Have evidence of appropriate academic qualifications and/or professional experience** demonstrating that the applicant has developed knowledge of the field of study or cognate field and the potential for research sufficient to undertake the chosen project.

AND

- Have **English level C1 language proficiency**.

In addition to the above, if your application is successful, you will be required to:

- Apply for a working visa in Spain (More information: http://www.exteriores.gob.es/Portal/en/ServiciosAlCiudadano/InformacionParaExtranjeros/Paginas/Requisito_sDeEntrada.aspx)
- Apply for a student visa in Australia (More information: <https://www.rmit.edu.au/study-with-us/international-students/apply-to-rmit-international-students/student-visas/apply-for-a-visa>)

In addition to meeting the eligibility criteria for the REDI Program, you will also need to meet the admission criteria of both institutions:

Admission at UAB

You will be enrolled as Doctoral Student at UAB for the entire duration of the assignment. At admission, you will need to supply:

- Degree certificate and the transcript of records of a Bachelor's degree and Master's degree (original and photocopy). Access may be granted where the following cases apply:
- Hold an official Spanish university degree or a degree from another country in the EEES which grants access to a Master's degree in accordance with article 16 of RD 1393/2007, of 29 October, and have achieved a minimum of 300 ECTS credits in university studies of which at least 60 must be at Master's level. In this case we must remember that the official university degree obtained correspondence to Level 2 of the Spanish Qualifications Framework for Higher Education (MECES), for official titles of Graduate or Engineer will be accounted for as a degree of 180 ECTS.
- Hold an official Spanish qualification at graduate level, the duration of which, in accordance with community law, must be at least 300 ECTS credits. These graduates must take compulsory background credit referred to

in article 7.2 of RD 99/2011, except where the syllabus of the degree course includes research training credits equivalent to the research credits awarded on Master's courses.

- University graduates who, before obtaining a place as a result of the entrance exam for specialist health courses, have passed at least two years of a programme for an official qualification in one of the Health Science specialisations.
 - Holder of a qualification obtained in accordance with foreign educational systems without the need for official recognition, having previously confirmed with the university that this qualification accredits a level of training equivalent to the official Spanish university Master's degree and that it would serve as a means of access to a PhD in the country in which it was awarded. This admission does not under any circumstances imply official recognition of the previous qualification or recognition for any purpose other than access to PhD studies.
 - Holders of another Spanish PhD qualification obtained in accordance with the previous university's rules.
 - Holders of a degree who also have the Diploma of Advanced Studies obtained in accordance with the provisions of RD 778/1998, of 30 April, or have achieved research proficiency under the terms outlined in RD 185/1985, of 23 January.
 - Hold an official university degree which has obtained correspondence to level 3 of the Spanish Qualifications Framework for Higher Education (MECES), for official degrees of Architect, Engineer or Bachelor.
- Cover Letter
 - CV including contact details
 - 2 reference letters
 - At the time of admission, the assignment of tutor, director and line of investigation will be necessary.
 - Admission to the PhD programme is decided by the Rector and depends on having passed the bridging courses, where they exist.

For those Candidates who have obtained their qualifications abroad formal requirements are needed to be followed to validate them. For more info, visit: <https://www.educacionyfp.gob.es/en/servicios-al-ciudadano/catalogo/general/20/203615/ficha.html>

More information: <https://www.uab.cat/web/study/phds/admission/admission-new-doctoral-studies-regulated-by-rd-99/2011-1345666996343.html>

Admission at RMIT University

You will also be enrolled as Doctoral Student at RMIT University for the entire duration of the assignment. At admission, you will need to supply:

- CV
- Complete transcripts for all academic qualifications
- Research proposal or statement of interest in an available research project
- Language certificates
- List of referees

More information: <https://www.rmit.edu.au/research/research-degrees/how-to-apply>

Apply now (<https://www.rediprogram.eu>)

