

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	01/01/2023 (tentative)
Deadline for applications	19/09/2022 (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
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.	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.	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.
Supervisors: <u>Prof. Pablo Ordejon (ICN2) and Ivan Cole (RMIT)</u>		
Research Fields: Corrosion; Density Functional Theory;	Research Fields: Corrosion; Density Functional Theory;	Research Fields: Corrosion; Density Functional Theory;



Molecular Modelling; Multiscale Modelling	Molecular Modelling; Multiscale Modelling	Molecular Modelling; Multiscale Modelling
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For more information on the Projects, contact us: redi.help@rmit.edu.au

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.

For more information about the general conditions of the REDI Program and the Eligibility Criteria, please visit: <https://www.rediprogram.eu/>

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>

Learn more on [RMIT](#), [ICN2](#), and [UAB](#) on our website: <http://www.rediprogram.eu/about/#hostinstitutions>



PhD enrolment. Successful candidates for this position will be enrolled by the following 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>

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