

## Position Description

### 1. General Information

Name of the position	<b>Accelerated Discovery of Supramolecular Molecular Energy Storage Systems</b>
Foreseen enrolment date	September 2025
Position is funded by	<ul style="list-style-type: none"> <li>• COFUND, Marie Skłodowska-Curie Actions (MSCA), Horizon Europe, European Union</li> <li>• Universitat Politècnica de Catalunya (UPC)</li> <li>• RMIT University</li> </ul>
Research Host	Universitat Politècnica de Catalunya (UPC)
PhD awarding institutions	Universitat Politècnica de Catalunya (UPC) & RMIT University
Locations	Primary: Barcelona, Spain Secondary: Melbourne, Australia
Salary	26,626.09 EUR annual <b>gross</b> salary (2,218.84 EUR monthly gross salary)
Supervisors	<ul style="list-style-type: none"> <li>• Kasper Moth-Poulsen, Professor, UPC</li> <li>• Josep Lluís Tamarit, Professor, UPC</li> <li>• Xavier Mulet, Professor, RMIT University</li> <li>• Tu Le, Dr., Senior Lecturer, RMIT University</li> </ul>
Group of discipline	Chemistry and Chemical Engineering

### 2. Research topics (only one of these projects will be funded)

#### Project 1: *Molecular Solar Thermal Management Materials*

This project seeks to fundamentally change how we generate heating and cooling by developing a new class of materials that capture, store, and release both solar and ambient heat. These solar thermal management materials are a unique combination of molecular photo-switches that capture and store solar energy, so-called MOST (molecular solar thermal) systems, that together with phase change materials (PCMs) can contribute to thermal management. The two classes of materials operate at fundamentally different principles. The input of MOST system is photons, and the output is heat whereas PCM can absorb heat from the environment. By combining the two materials into one, we can harness and upgrade two of the most abundant renewable sources of energy on the planet: ambient heat and sunlight. The MOST systems are based on so-called photoswitches, that are molecules that undergo isomerisation upon exposure to light. Examples include Norbornadiene-Quadricyclane couple, the Azobenzene Z/E isomerisation and Anthracene dimerization. The



work with include organic synthesis, physical characterisation, accelerated discovery methods and testing in devices.

**Supervisors:** Kasper Moth-Poulsen (UPC), Josep Lluís Tamarit (UPC), Xavier Mulet (RMIT)

**Research Fields:** Materials Science and Engineering, Renewable Energy Technologies

### **Project 2: Molecular Solar Thermal Management Materials: flow synthesis and accelerated discovery**

This project seeks to fundamentally change how we generate heating and cooling by developing a new class of materials that capture, store, and release both solar and ambient heat. These solar thermal management materials are a unique combination of molecular photo-switches that capture and store solar energy, so-called MOST (molecular solar thermal) systems, that together with phase change materials (PCMs) can contribute to thermal management. The two classes of materials operate at fundamentally different principles. The input of MOST system is photons, and the output is heat whereas PCM can absorb heat from the environment. By combining the two materials into one, we can harness and upgrade two of the most abundant renewable sources of energy on the planet: ambient heat and sunlight. The MOST systems are based on so-called photoswitches, that are molecules that undergo isomerisation upon exposure to light. Examples include Norbornadiene-Quadricyclane couple, the Azobenzene Z/E isomerisation and Anthracene dimerization. This project will focus on molecular design and synthesis of the molecular photoswitch systems with goal of developing photoswitchable phase change materials with synergistic interplay with traditional phase change materials.

**Supervisors:** Kasper Moth-Poulsen (UPC), Josep Lluís Tamarit (UPC), Xavier Mulet (RMIT)

**Research Fields:** Energy Materials and Thermal Energy Storage, Photochemistry

### **Project 3: Molecular Solar Thermal Management Materials: accelerated discovery of new supramolecular systems**

This project seeks to fundamentally change how we generate heating and cooling by developing a new class of materials that capture, store, and release both solar and ambient heat. These solar thermal management materials are a unique combination of molecular photo-switches that capture and store solar energy, so-called MOST (molecular solar thermal) systems, that together with phase change materials (PCMs) can contribute to thermal management. The two classes of materials operate at fundamentally different principles. The input of MOST system is photons, and the output is heat whereas PCM can absorb heat from the environment. By combining the two materials into one, we can harness and upgrade two of the most abundant renewable sources of energy on the planet: ambient heat and sunlight. The MOST systems are based on so-called photoswitches, that are molecules that undergo isomerisation upon exposure to light. Examples include Norbornadiene-Quadricyclane couple, the Azobenzene Z/E isomerisation and Anthracene dimerization. This project will focus on exploring the interaction and properties of mixtures of advanced photoswitchable phase change materials with traditional phase change concepts. Large composition structure-property materials space will be explored using a combination of traditional physical chemistry tools such as microscopy and differential scanning calorimetry (DSC) as well as the newly established robotized research platform at UPC that allow for accelerated creation of supramolecular materials libraries. For the use of the robotized platform a special interest in programming and robotics will be needed.



**Supervisors:** Kasper Moth-Poulsen (UPC), Josep Lluís Tamarit (UPC), Xavier Mulet (RMIT)

**Research Fields:** Thermal Energy Management and Engineering Computational Material Science, Chemistry

### 3. Employment Benefits and Conditions

Universitat Politècnica de Catalunya (UPC) offers a 48-month full time work contract. The total working hours per week are 37.5.

The remuneration, in line with the European Commission rules for Marie Skłodowska-Curie grant holders, will consist of a **gross annual salary** of yearly 26,626.09 EUR (which is of monthly 2,218.84 EUR). Of this amount, the estimated net salary to be perceived by the Researcher is 1,819.00 EUR per month. However, the definite amount to be received by the Researcher is subject to national tax legislation and the personal situation.

#### Benefits include

- Becoming a Marie Skłodowska-Curie fellow and be invited to join the Marie Curie Alumni Association
- Access to all the necessary facilities at UPC and RMIT University
- Tuition fees exemption at both PhD awarding institutions
- Travel allowance to cover flights and accommodation for participating in DREAM+PLAN events
- Up to 12 months in Australia
- 22 days paid holiday leave
- Social security coverage
- Sick leave
- Parental leave

### 4. PhD enrolment

Successful candidates for this position will be enrolled by the following institutions and must comply with their specific entry requirements, in addition to DREAM+PLAN's conditions.

#### Universitat Politècnica de Catalunya (UPC)

To enrol in a Doctorate program you must meet the general conditions, namely:

As a rule, applicants seeking admission to an official doctoral programme must hold a Spanish bachelor's degree or equivalent and a Spanish master's degree or equivalent, provided they have passed at least 300 ECTS credits on the two degrees. Any of the following applicants may also gain admission:



- Holders of official Spanish degrees or equivalent Spanish qualifications, provided they have passed 300 ECTS credits in total and they can prove they have reached Level 3 in the Spanish Qualifications Framework for Higher Education.
- Holders of degrees awarded in foreign education systems in the European Higher Education Area (EHEA), which do not require homologation, who can prove that they have reached Level 7 in the Spanish Qualifications Framework for Higher Education, provided the degree makes the holder eligible for admission to doctoral studies in the country in which it was awarded. Admission on this basis does not imply homologation of the foreign degree or its recognition for any purpose other than admission to doctoral studies.
- Holders of degrees awarded in a country that does not belong to the European Higher Education Area, which do not require homologation, on the condition that the University is able to verify that the degree is of a level equivalent to that of official university master's degrees in Spain and that it makes the graduate eligible for admission to doctoral studies in the country in which it was awarded. Admission on this basis does not imply homologation of the foreign degree or its recognition for any purpose other than admission to doctoral studies.
- Holders of another doctoral degree.
- University graduates who, having previously been awarded a training post in the entrance examination for specialised health training posts, have passed and obtained a positive assessment in at least two years of training on a programme leading to an official qualification in a Health Sciences specialisation.

Specific requirements and admission procedure:

Each doctoral programme may have specific requirements for admission in addition to the general requirements. The additional specific requirements that must be met for admission are listed on the web pages for each programme.

More information: [https://doctorat.upc.edu/en/future-doctoral-candidates/access-and-admission/general-entrance-requirements?set\\_language=en](https://doctorat.upc.edu/en/future-doctoral-candidates/access-and-admission/general-entrance-requirements?set_language=en)

### **RMIT University**

Visit the website: <https://www.rmit.edu.au/research/research-degrees/how-to-apply>

