AUFRANDE ICMPE Institut de Chimie et des Matériaux Paris-Est UNSW SYDNEY

Position Description

1. General Information

Name of the position	**Polymer-ionic liquid composites for Li(Na) batteries: toward new polymer-based solid electrolytes**
Foreseen Enrolment date	1 October 2023
Position is funded by	• COFUND, Marie Skłodowska-Curie Actions (MSCA), Horizon Europe, European Union • Institut de Chimie et des Matériaux Paris-Est (ICMPE/UPEC-CNRS) • The University of South Wales (UNSW) Sydney
Research Host	Institut de Chimie et des Matériaux Paris-Est (ICMPE/UPEC-CNRS)
PhD awarding institutions	Université Paris-Est Créteil (UPEC) & University of New South Wales (UNWS)
Locations	Primary: Thiais, France Secondary: Sydney, Australia
Supervisors	Dr. Rita Baddour-Hadjean (ICMPE/UPEC-CNRS), Dr. Jean-Pierre Pereira-Ramos (ICMPE/UPEC-CNRS), Dr. Thi-Thanh-Tam Nguyen (ICMPE/UPEC), Dr. Daniel Grande (ICMPE/UPEC-CNRS) Dr. Dipan Kundu (UNSW)
Group of discipline	Energy storage, Li (Na) batteries, Chemistry, Polymer science, Materials science, Solid-state chemistry, Electrochemistry

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

Project 1: *Polymer-ionic liquid composites for lithium-ion batteries: toward new polymer based solid electrolytes*
The proposed project concerns the synthesis of new solid electrolyte membranes based on thermostable polymers and ionic liquids (ILs) for being used as ion-conducting membranes in lithium-ion batteries (LIBs). The originality of this approach lies in the use of polycyanurates (PCNs), a family of thermosetting polymers with unique intrinsic properties (high chemical and thermal resistance, low dielectric constant and strong adhesion to conductive metals and composites) as polymer matrix for impregnating ILs. These polymers have mainly been used as binders in high performance structural composites, especially in the aeronautical and aerospace industry but have not been exploited in the microelectronics industry yet because of their brittleness while suitable polymer materials used in microelectronic devices must be flexible. Recently, we have found that the presence of a small amount of ILs during the step of forming PCN networks

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produces flexible conductive PCN-ILs membranes that could replace both microporous separators and flammable volatile organic electrolytes in Li-ion batteries. Indeed, thanks to the presence of nano-domains containing ILs, these membranes would facilitate the mobility of Li^+ cations while maintaining the electronic insulation even at a high temperature. They would also act as a physical barrier against dendritic growth, hence reducing the risk of short circuit, thermal runaway, explosion and thus significantly improving the safety of LIBs and therefore would enable to replace conventional anodic materials, *i.e.* graphite, by metallic lithium one for producing metallic lithium batteries (MLBs) with very high energy density. It is noteworthy to mention that the impregnation of ILs would endow the membranes with the ionic conductivity with improved safety issues thanks to the non-volatility, non-flammability and no leakage of impregnated ILs. Moreover, recent studies show that the use of ILs can significantly increase the electrochemical properties of a solid-state battery, such as improving the long-term stability of lithium metal electrodes and the interfacial compatibility with electrodes. The main objective of this PhD project will be the development of high-performance ion-conducting membranes based on PCNs/ILs composites for being used in LIBs and MLBs.

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Research Fields: Energy storage, Li batteries, ionic liquids, Polymer science, Materials science, Solid-state chemistry, Electrochemistry

Project 2: *Thermostable polymer/IL composites for applications in next generation Na-ion batteries*

Among the various types of electrochemical energy storage technologies, Li^+-ion batteries are still in the forefront and are currently playing an indispensable role in supporting our modern society. Electrochemistry of lithium-based cell presents various attractive properties: i) lithium is the lightest metal with an exceptional low redox potential ($E_{Li+/Li} = -3.04$ V/NHE); ii) Li^+-ion possesses a small ionic radius that is advantageous for easy diffusion into solid; iii) Li^+-ion based cell has a long cycle life with high rate capability *etc*. Unfortunately, lithium resources are limited: only 20 ppm as relative abundance in the Earth's crust. Thus, many researchers try to explore new abundant and low-cost alternatives to lithium such as sodium, potassium or calcium. Sodium is cheap, available in a high abundance (1000 times more abundant than lithium) with very desirable redox potential, *i.e.* $E_{Na+/Na} = -2.71$ V/NHE, only 0.3 V greater than that of lithium, and similar electrochemical behaviour. The proposed project concerns the synthesis of new solid electrolyte membranes based on thermostable polymers and ionic liquids (ILs) for being used as ion-conducting membranes in sodium-ion batteries (SIBs). The originality of this approach lies in the use of polycyanurates (PCNs), a family of thermosetting polymers with unique intrinsic properties (high chemical and thermal resistance, low dielectric constant and strong adhesion to conductive metals and composites) as polymer matrix for impregnating ILs. These polymers have been mainly used as binders in high performance structural composites, especially in the aeronautical and aerospace industry but have not yet been exploited in the microelectronics industry because of their brittleness. Recently, we have found that the presence of a small amount of ILs during the step of forming PCN networks produces flexible conductive PCN-ILs membranes that could replace both microporous separators and flammable volatile organic electrolytes in Li-ion batteries. Indeed, the presence of nano-domains containing ILs within these membranes would facilitate the mobility of Na^+ cations while maintaining the electronic insulation even at a high temperature. They should act as a physical barrier against dendritic growth, hence reducing the risk of short circuit, thermal runaway, explosion and thus, significantly improving the safety of Na-ion batteries and therefore would enable to replace conventional graphite based anode by metallic sodium for producing batteries with very high energy density. The impregnation of ILs would endow the membranes with ionic conductivity with improved safety issues thanks to the non-volatility, non-flammability and no leakage of impregnated ILs. Recent studies show that the use of ILs can significantly increase the electrochemical properties of a solid-state battery, such as improving the long-term stability of metal electrodes and the interfacial compatibility with electrodes.

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Research Fields: Energy storage, Na-ion batteries, Polymer science, Ionic liquids, Materials science, Solid-state chemistry, Electrochemistry

Project 3: *Ionic liquids-biosourced polymer based composites meant for sustainable Li-ion batteries*
The proposed project concerns the synthesis of high-performance solid electrolyte membranes based on biosourced thermostable polymers and ionic liquids (ILs) for being used as ion-conducting membranes in lithium-ion batteries (LIBs). The originality of this approach lies in the use of biosourced polycyanurates (PCNs), a family of thermosetting polymers with unique intrinsic properties (high chemical and thermal resistance, low dielectric constant and strong adhesion to conductive metals and composites) as polymer matrix for impregnating ILs. These polymers have mainly been used as binders in high performance structural composites, especially in the aeronautical and aerospace industry but have not been exploited in the microelectronics industry yet because of their brittleness. Recently, we have found that the presence of a small amount of ILs during the step of forming PCN networks produces flexible conductive PCN-ILs membranes that could replace both microporous separators and flammable volatile organic electrolytes in Li-ion batteries. Indeed, thanks to the presence of nano-domains containing ILs, these membranes would facilitate the mobility of Li^+ cations while maintaining the electronic insulation even at a high temperature. They would also act as a physical barrier against dendritic growth reducing the risk of short circuit, thermal runaway, explosion and thus significantly improving the safety of LIBs and therefore would enable to replace conventional graphite based anode by metallic sodium for producing batteries with very high energy density. It is worth mentioning that biosourced PCNs will be designed and synthesized from renewable starting materials, thus avoiding the use of toxic bisphenol E. The impregnation of ILs endows the membranes with the ionic conductivity with improved safety issues owing to the non-volatility, non-flammability and no leakage of impregnated ILs. Moreover, recent studies have shown that the use of ILs can significantly increase the electrochemical properties of a solid-state battery, such as improving the long-term stability of lithium metal electrodes or the interfacial compatibility with electrodes.
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Research Fields: Energy storage, Li batteries, sustainable developments, ionic liquids, Polymer science, Materials science, Solid-state chemistry, Electrochemistry

3. Employment Benefits and Conditions

The Institut de Chimie et des Matériaux Paris-Est (ICMPE) - Université de Paris-Est Créteil (UPEC) / Centre National de la Recherche Scientifique (CNRS) offers a 36-months full-time work contract (with the option to extend up to a maximum of 42 months). A probation period of 2 month will apply. The legal working time is 38 h and 40 min 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 28,800 EUR. Of this amount, the estimated net salary to be perceived by the Researcher is 1,850 EUR per month. However, the definite amount to be received by the Researcher is subject to national tax legislation.

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Benefits include

- Access to all the necessary facilities and laboratories at ICMPE – UPEC/CNRS and UNSW.
- Tuition fees exemption at both PhD awarding institutions.
- Yearly travel allowance to cover flights and accommodation for participating in AUFRANDE events.
- 10,000 EUR allowance to cover flights and living expenses for 12 months in Australia.
- 45 days paid per year holiday leave.
- Affiliation to the French social security system and its legislation on accidents at work.

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 AUFRANDE's conditions.

UPEC

To be eligible to apply for a PhD a Master's degree Diploma or equivalent qualification is needed.

Approval of the CNRS defence security officer may be required before the starting of employment. In case of denial, the employment will not be carried out.

More information: https://www.paris-est-sup.fr/ecoles-doctorales/ecole-doctorale-sciences-ingenierie-et-environnement-sie/accueil/

UNSW

The minimum entry requirement for admission to a PhD includes:

- an appropriate UNSW bachelor degree with upper second-class honours; or
- a completed Masters by Research from UNSW with a substantial research component and demonstrated capacity for timely completion of a high-quality research thesis; or
- an equivalent qualification from a tertiary institution as determined by the Faculty Higher Degree Committee (HDC).

If English is not your first language, you will be required to provide evidence your English language proficiency. Note that your English test needs to be completed no more than two years before your enrolment at UNSW. The English language test scores requirements can be found here: https://www.unsw.edu.au/study/how-to-apply/english-language-requirements

More information: https://research.unsw.edu.au/higher-degree-research-programs

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