INDUSTRIAL PARTNERSHIP
MASTER'S DEGREE THESIS



GES

Reshaping the energy transition

Project #004 dated:
September 15th, 2022

Proposal available until:
December 23rd, 2022

Email hr@greenenergystorage.eu
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THESIS PROJECT

CALCULATION OF SOLVATION FREE ENERGIES OF ORGANIC SOLUTES VIA AB-INITIO MOLECULAR DYNAMICS METHODS

OVERVIEW

Field
Computational chemistry

Duration
6 months

Degree course
Master's Degree

REDOX FLOW BATTERIES

Redox Flow Batteries (RFBs) are secondary batteries mostly used for energy storage applications. These systems work very well with renewable energy sources during charge, they store energy for a later use, when they can be discharged.

Compared to other electrochemical energy storage technologies, RFBs store energy in the anolyte and catholyte tanks outside the cell, where redox reactions occur. Energy is therefore defined by the amount of electrolyte in the tanks, while power is defined by the size of the cell. This unique feature of decoupled energy and power enables the flexibility to independently adjust battery power and energy to achieve large scale energy storage systems. In addition, redox flow batteries boast a very high number of cycles compared to other battery systems.

THE CHALLENGE OF ORGANIC ELECTROLYTES

Particular attention in the field of research is now paid to the development of RFBs based on organic electrolytes, thanks to the possibility of engineering their molecular structure to maximize properties such as solubility and redox potential, as well as the abundance of available raw materials.

A strong push in the discovery of new organic electrolytes comes from the use of computational methods, which allow us to predict key properties of compounds such as the redox potential, in order to identify the most promising molecules without the need to synthesize and test their performance in a laboratory. Numerous studies have been published on the calculation of redox potential using quantum mechanical methods[1–3], but their applicability is limited by the difficulty of realistically reproducing the interactions between the electrolyte and the solvation medium.



HOW TO APPLY

Contacts and useful informations

Applications can be sent to mattia.palermo@greenenergystorage.eu

Please attach a motivation letter and a short CV

For technical question, reach out to:

Luca Babetto
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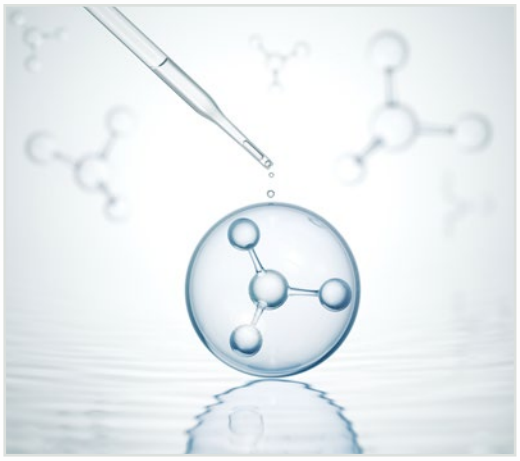
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THE RESEARCH PROJECT

The proposed research project aims to evaluate the accuracy of ab-initio molecular dynamics simulations in describing the interaction between organic species and the aqueous solvent. Implicit solvation methods commonly used in electronic structure simulations to approximate the solute-solvent interaction are in fact unable to realistically describe systems containing charged species[4], which are instead typically present in redox processes. The inability to correctly estimate the energetics of the solvation process in turn leads to non-negligible errors in the prediction of the redox potential of organic electrolytes, therefore preventing the widespread application of computational methods for the design and screening of novel electrolytes. Such limitation is particularly true for engineered high-performance electrolytes, whose chemistries intrinsically rely on highly charged species. In fact, high energy densities are typically achieved by functionalization of molecular scaffolds with charged functional groups to increase solubilities, and whose redox center of reaction are chosen so that it undergoes a multielectron redox process.



In this research project, the accuracy of ab-initio molecular dynamics simulations of explicitly solvated species will be determined through the calculation of the free solvation energy for neutral and ionic organic solutes. The technique will be validated through the comparison of the calculated free energy of solvation with the experimental evidence from datasets of free solvation energies available in the literature[4]. A comparison of developed method with state-of-the-art implicit solvation methods will also be performed in order to evaluate its effectiveness, both in terms of accuracy and required computational resources.

References

1) Zhang, Q., Khetan, A., & Er, S. (2020). Scientific Reports, 10(1) 1–13.

2) Neugebauer, H. et al(2020). The Journal of Physical Chemistry A, 124(35), 7166–7176

3) Maier, S., Thapa, B., & Raghavachari, K. (2020). Phys. Chem. Chem. Phys., 22(8), 4439–4452

4) Marenich, A. V., Cramer, C. J., Truhlar D. G. (2009). J. Phys. Chem. B 2009, 113, 18, 6378–6396

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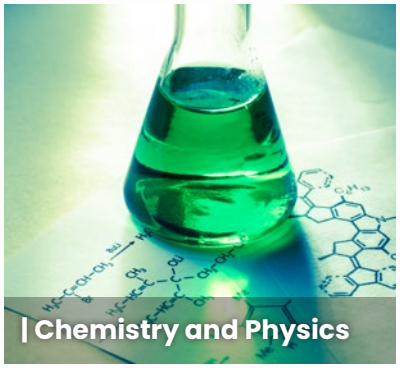
YOUR THESIS

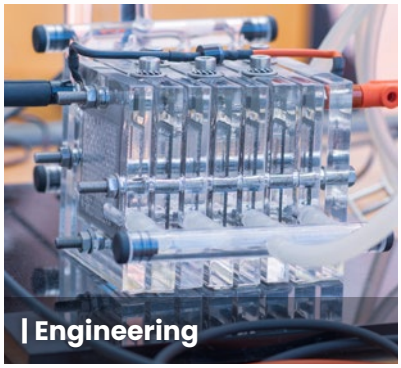
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- Your thesis research will be supported by our industrial tutor
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THESIS IN GES

Part of the thesis research project might be carried out at GES labs and facilities, depending on the research topic and the specific industrial needs





YOU HAVE A THESIS IDEA OR WANT TO KNOW MORE ABOUT AVAILABLE OPPORTUNITIES

Get in touch with us at hr@greenenergystorage.eu

YOUR THESIS

GES

Green Energy Storage (GES) is an SME specialized in the development of Redox Flow Batteries.

Developing the energy storage of the future with the supply chain in mind: we develop green chemistries based on abundant, readily available materials with a low environmental impact

VISION

Thanks to a new technology based on hydrogen and a hydrib gas/liquid platform, GES aims at developing next-gen electrochemical storage technologies that are non-toxic, inherently safe, composed by readily available materials at a competitive price and operating at ambient temperature.

GES was granted a 53 millions euro fund from the European Union and the Italian Government for the IPCE Battery 2 project, focused on the research and development of innovative solutions for the whole battery value-chain, with a strong focus on the environmental sustainabilty.

THE (WORK) ENVIRONMENT IS OUR STRENGTH



What sets us apart

- A young and dynamic company located at the heart of the Alps.
- A highly qualified research team composed by 50% of PhDs in Physics, Chemistry and Computational Chemistry.
- 20 people, 11 countries: GES is a place of technological frontier, where talents with experience from different contexts of international excellence meet to shape the future of the energy storage

GES

WORK WITH US FOR THE FUTURE OF ENERGY



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Work with us:

Apply for one of the open positions or send an unsolicited application. Our team is always look for new talents.