

## **On the quest for new RFB redox couples: a computational approach**

Redox Flow Batteries (RFBs) are one of the most promising electrochemical storage technologies that, once coupled to intermittent renewable energy sources, will allow for a constant and resilient energy supply. While vanadium-based, commercial RFB technologies have been under development since the '80s, new electrolyte classes are being explored to improve the energy storage performance and reach the target set by the European Strategic Energy Technology (SET) Plan [1]. In recent years, screening techniques based on quantum chemical methods have been employed to accelerate the design of electroactive compounds. In this talk, I will present some of the state-of-the-art applications of these methods for the prediction of key properties such as redox potential, solubility, and stability of organic electrolytes. I will also cover the unsolved challenges in the field and some of the most recent advances that could further push the accuracy and applicability of these techniques, with a particular focus on how this approach can also be applied in an industrial context.

### References

[1] "SET Plan delivering results: The Implementation Plans", Publications of the European Union 2018, DOI 10.2833/25250