HORIZON 2020

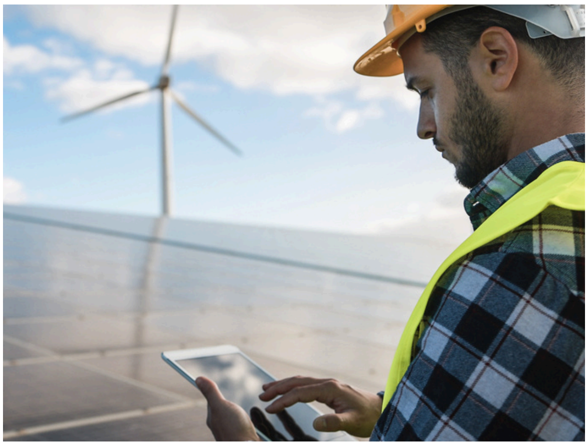
Modelling for the search for new active materials for redox flow batteries

Results in Brief

Computational approach to achieving greener batteries

New computational methods for identifying viable organic battery materials could help Europe to establish a greener, more sustainable energy supply chain.

ENERGY



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Concerted efforts are under way to increase the amount of renewable energy available to the grid. To ensure this is successful, new ways for storing this energy are required, to compensate for times where there is no wind or little sun.

One technology that has shown potential here is redox flow batteries (RFBs). Energy is stored in liquid, and can be released when demand increases. This could help make renewable energy sources more adaptable to the needs of the grid.

Optimising identification of organic materials

"A key challenge however is that most materials used to make RFBs – metals such as vanadium – are not available in the EU," notes SONAR project coordinator Jens Noack from the Fraunhofer Society in Germany. "We need to find abundantly available organic materials if we are to develop a sustainable energy supply."

The goal of the EU-funded SONAR project was therefore to find ways of optimising the identification of viable abundant organic materials, which could then be used to make RFBs. To do this, the project brought together academic institutions as well as industrial partners, material producers and computational experts.

The project applied computational methods to achieve high-throughput screening of potential material candidates. “This was the motivation – to speed up the research process by conducting initial screenings by computer,” explains Noack. “Promising candidates can then be synthesised in the lab.”

Linear high-throughput screening approach

Online demonstrators were developed, and made freely available in order to highlight the potential of this computational approach. Various components and models were developed and can be combined to create a linear, high-throughput screening approach.

“We developed demonstrators to work at different scales and address different issues,” adds Noack. “We start at the quantum scale, then at the electrode scale, and go all the way up to grid scale.”

The computational approaches pioneered by SONAR also cover estimating electrode reactions, which account for most energy and efficiency losses, as well as site reactions.

“All these things need to be considered,” says Noack. “If we can identify potential site reactions from the beginning, then we know that a particular material will not be economically viable.”

Other economic models were devised, enabling developers to calculate the potential cost of using particular RFB materials at the grid level. “The ultimate determining factor is overall cost,” notes Noack.

Identifying organic, abundantly available materials

The high-throughput screening means that users can carry out real-time screening of potential organic materials, without the need for lab testing.

Noack believes that computational modelling at the quantum scale will mostly likely appeal to academics and researchers, looking to push the boundaries of knowledge. Techno-economic analytical models meanwhile will be of most interest to industry, keen to see what materials are most likely to be commercially viable.

The SONAR project has achieved both, and developed a modular, high-throughput process that can now be used to identify organic, abundantly available materials. “The next step is to start looking for candidates,” adds Noack. “This is what we are now planning to do.”

Keywords

SONAR batteries redox flow batteries energy organic redox quantum electrode

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