them.

HighMag

The Magnesium Charge

Big Instruments for Small Problems: Using Large Research Facilities to Study Magnesium Batteries

Magnesium: A Promising Energy Storage Material

Although Li-ion batteries dominate the current energy storage market, there are serious limitations in the availability of critical materials used in these batteries such as cobalt, nickel, and Li itself. To fill this gap, the European Union's Horizon Europe program funded HighMag, a four-year research project. HighMag brings together 13 industrial and academic partners to investigate next-generation, non-Li-based batteries.

The HighMag project focuses on magnesium-based batteries where the divalent Mg2+ ions act as the charge carrier rather than Li+ ion, which are used in Li-ion batteries. Moreover, we utilize magnesium manganese oxide (MMO) and sulphur (S) cathodes and Mg metal as the anode. None of these materials suffer from the same supply chain limitations that Li-ion batteries do and therefore offer a promising pathway towards more sustainable energy storage devices.

"For the HighMag project, the Paul Scherrer Institute uses the Swiss Light Source (SLS) to conduct X-ray diffraction (XRD), X-ray absorption spectroscopy (XAS) and X-ray Computed Tomography (X-CT) experiments on Mg batteries."

Charles Soulen
Post-doctoral researcher at the Paul Scherrer Institute. Specialized in the utilization of advanced characterization techniques to study Li-ion, Li-metal, Mg-metal, and Li all-solid-state batteries.

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Mg batteries have other practical characteristics which makes them attractive to researchers. First, in a battery, Mg becomes an Mg2+ ion, giving it the ability to transfer two electrons compared to Li's one. Therefore, Mg batteries could provide significantly higher charge per volume compared to Li batteries. Second, the production and recycling of Mg metal is already an industrial process. The commercial Mg batteries could be integrated into an existing supply chain, significantly improving the possibility of widespread adoption. The recyclability of Mg offers further benefits to the sustainability of this technology.

Despite these advantages, Mg batteries still require further development. Significant challenges remain on both the MMO and S cathodes, and the Mg metal anode. Regarding the MMO cathode, a more comprehensive understanding of the crystallographic changes which occur during charge and discharge is essential. Such insights will support the design of new cathode materials that can mitigate structural degradation during cycling. In magnesium–sulfur (Mg–S) batteries, the mechanisms governing polysulfide formation and shuttling need to be elucidated. The Mg metal anode present additional challenges. A deeper understanding of the mechanisms and special distribution of Mg plating and stripping during cell operation is needed to limit capacity loss and mitigate cell failure. Finally, we aim to characterize the interfaces between the anode, cathodes, and electrolytes developed for HighMag. Unstable interfaces can lead to capacity loss, and premature cell failure. Addressing these questions requires advanced, multimodal characterization capabilities capable of probing structural, chemical, electrochemical, and morphological changes under realistic operating conditions. At the Paul Scherrer Institute (PSI), we have extensive expertise in the large research facilities (LRF) necessary to answer these questions.

The Paul Scherrer Institute and its Facilities:

At the Paul Scherrer Institute (PSI), we develop and operate some of Switzerland's most advanced research facilities. These facilities use powerful beams of X-rays, neutrons, muons, and other particles to study materials and processes that are important for energy, climate, health, and many other fields. Every year, more than 2,000 researchers from around the world come to PSI to use these unique facilities.

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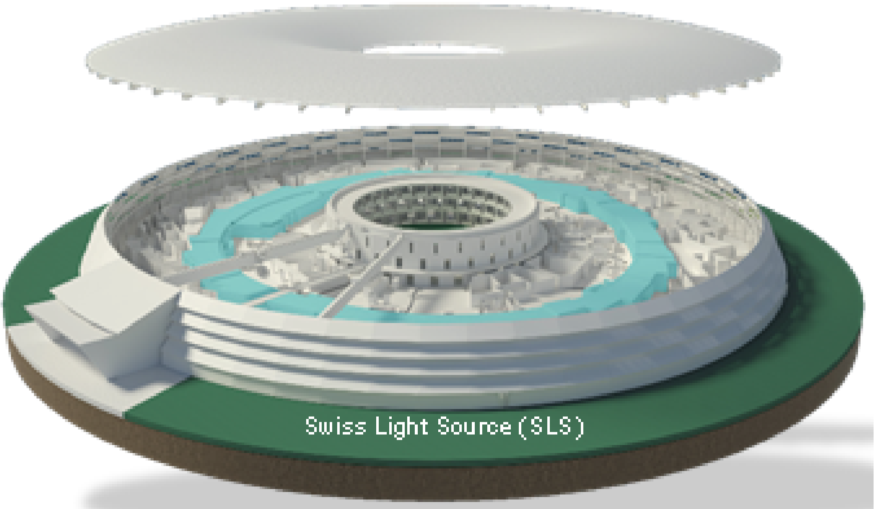
One of PSI's key facilities is the **Swiss Light Source (SLS)**, a large research facility that produces very bright X-ray beams. These X-rays allow scientists to look inside materials and batteries and understand how they change during operation.

HighMag and the Swiss Light Source

In the **HighMag project**, we will use the SLS to study Mg batteries. Different X-ray techniques will allow us to investigate how the battery materials change during operation. This information will help us understand why Mg batteries degrade and how they can be improved.

The SLS works by accelerating electrons to very high speeds and circulating them around a large storage ring. Powerful magnets guide the electrons around the ring and generate intense X-ray light. This X-ray light is directed through dedicated experimental stations, called beamlines, where researchers use it to study different materials.

The SLS therefore acts like a powerful scientific "camera", allowing us to look inside working batteries without taking them apart. By using this unique capability, HighMag aims to provide new knowledge that can help advance Mg batteries toward future practical applications.



A diagram of the SLS
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X-ray Diffraction, X-ray absorption spectroscopy, and X-ray Computed Tomography

The HighMag team at PSI will use the Swiss Light Source (SLS) to study Mg batteries with three complementary X-ray techniques: X-ray diffraction (XRD), X-ray absorption spectroscopy (XAS), and X-ray computed tomography (XCT). Together, these techniques allow us to look at batteries at different scales, from individual atoms to the overall structure of the battery and understand what happens while the battery is charging and discharging.

X-ray diffraction (XRD) helps us understand how the atoms in the battery materials are arranged. We will use XRD to study the MMO materials used as positive electrodes. When X-rays interact with these materials, they produce a characteristic pattern that acts like a fingerprint of their structure. By following how this pattern changes during battery operation, we can see how the atoms move and how the crystal structure changes as magnesium ions enter and leave the material. This will help us understand capacity loss and guide the development of more stable and higher-performing cathodes.

X-ray absorption spectroscopy (XAS) provides information about the chemical changes taking place inside the battery. By changing the energy of the X-ray beam, we can study specific elements and determine how their chemical state and surroundings change during charging and discharging. This allows us to follow chemical reactions that may be difficult to observe using other techniques, including polysulfide shuttling and those occurring at the interfaces between the battery materials and the electrolyte.

X-ray computed tomography (XCT) allows us to look inside a working battery in three dimensions. Similar to a medical CT scan, the battery is rotated while many X-ray images are recorded. These images are then combined to create a 3D picture of the battery. With XCT, we can observe how magnesium metal deposits and dissolves during cycling and identify structural changes such as cracks, voids, or uneven metal growth.

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Conclusion

XRD, XAS, and XCT are three powerful techniques which provide complementary views of how Mg batteries work and degrade. By connecting changes at the atomic and chemical levels with larger structural changes, HighMag aims to identify the causes of battery failure and develop safer, longer lasting Mg batteries. Through projects like HighMag, Europe leads the way in building a sustainable future.

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