2025 Helmholtz – OCPC – Program

for the involvement of postdocs in bilateral collaboration projects

PART A

Title of the project:

Designing high-performance cathode materials for sustainable magnesium-/calcium batteries

Helmholtz Centre and/or institute:

Karlsruhe Institute of Technology (KIT), Helmholtz Institute Ulm (HIU)

Project leader:

Prof. Maximilian Fichtner, Dr. Zhirong Zhao-Karger

Contact Information of Project Supervisor: (Email, telephone)

Phone: +49-731-50-34201 (M. F.), +49-721-608-28908 (Z. Z.)
Email: m.fichtner@kit.edu (M. F.), zhirong.zhao-karger@kit.edu (Z. Z.)

Web-address:

https://www.kit.edu/english/

Department: (at the Helmholtz centre or Institute)

Helmholtz Institute Ulm Electrochemical energy storage (HIU)

Program Coordinator (Email, telephone)

Name: Oliver Kaas
Phone: +49-721-608-45323
Email: oliver.kaas@kit.edu

Description of the project (max. 1 page)**:**

The commercialization of lithium-ion batteries (LIBs) and their drastic increasing market share in the energy sector has demonstrated the feasibility of utilizing rechargeable batteries towards decarbonization. However, the global demand for battery technology towards large-scale production has raised critical concerns regarding safety, cost, sustainability and robust material supply chains, which can hardly be addressed by the current LIBs alone. Therefore, advancing sustainable and cost-efficient so-called "post-lithium" battery systems could potentially provide alternative and complementary energy storage solutions, and enrich the application scenarios of power batteries, thereby effectively relieving the pressure on the resources for LIBs.

Rechargeable batteries utilizing divalent metal anodes, such as magnesium (Mg) and calcium (Ca), exhibit great promises of providing high energy density and safer cycling at a reduced cost, which are key criteria for battery applications. Compared with lithium, the divalent metal elements are more abundant and easier recyclable, making the respective system well suitable for massive production and sustainable implementation. A high-performance divalent metal battery relies on the efficient and reversible shuttling of the divalent ions (Mg-ions or Ca-ions) between the cathode and the metal anode. However, due to the bivalent nature of the charge carriers, their transport in cathode materials is generally hindered by strong interaction with the host lattice. Consequently, lack of suitable cathode materials that enable sufficient ion mobility without compromising with energy density is currently the most critical roadblock, which impedes the realization of practical divalent batteries.

To tackle these critical roadblocks, a Post Doc project in the framework of the Helmholtz-OCPC-Programme is proposed. The main focus of the project is to investigate the charge storage principle and kinetic behaviour of the divalent Mg-/Ca-ions, and from which further identifying key factors limiting the insertion kinetics of the charge carriers. For this purpose, advanced *in situ/operando* characterization techniques will be applied to uncover the evolution of crystal/electronic structures, the change of chemical compositions, and the dynamics in oxidation states etc. Based on the outcome, novel cathode materials that ideally operates at high voltages shall be developed, and tested electrochemically under realistic operation conditions.

The project is based on the expertise of the Fichtner/Zhao-Karger group at KIT-HIU/INT in the field of Mg-/Ca batteries. For more than 10 years, the group have been leading or participating in several EU-/national collaborative projects, which result in the development of the state-of-the-art electrolytes, novel sulphur-/organic cathodes, and alloy anodes etc. In addition, the group have access to advanced characterizations required for the current project, including X-ray Absorption Spectroscopy (XAS), X-ray diffraction (XRD), Raman-/Infrared spectroscopy etc. that can be operated *in situ/operando.*

Description of existing or sought Chinese collaboration partner institute (max. half page)**:**

The collaboration with the Chinese partner, the Qingdao Institute of Bioenergy and Bioprocess Technology (QIBEBT), the Chinese Academy of Sciences (CAS) as one of the leading institutes in China, is already well established in the field of Mg-/Ca batteries. The collaboration is based on a former postdoc Dr. Zhenyou Li in the Fichtner group, who left for China in 2023 and built an independent research group at QIBEBT working on multivalent batteries. With mutual benefits, the present collaboration with QIBEBT will deepen the exchange of know-how between the project partners in the field of cathode materials for alkaline-earth metal batteries and advanced characterizations by *in situ/operando* spectroscopic techniques. Based on that, further efforts will be made on acquiring collaboration projects between the two partners.

Required qualification of the postdoc:

- PhD in materials science, chemistry or a relevant discipline
- Experience with inorganic material synthesis and electrochemical measurements
- Additional skills in *in situ/operando* spectroscopy
- Fluent verbal and written English skills are required.