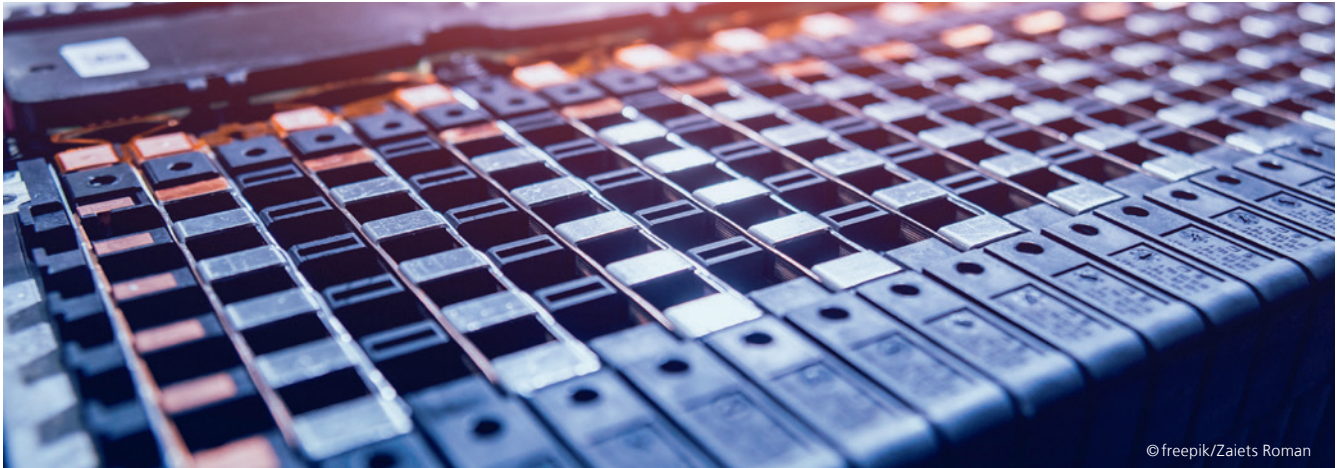


# DEFACTO – E-Mobility Gains at the Cellular Level Are Picking up Speed



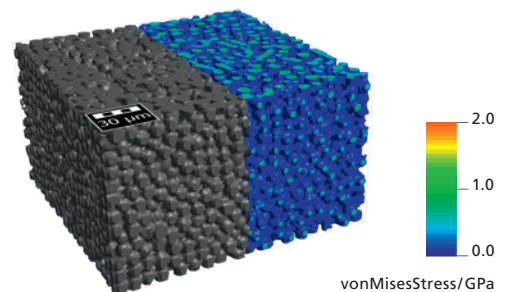
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## Revolutionizing European battery cell production

The EU’s DEFACTO project has set an ambitious goal: to develop a modeling tool-chain for e-mobility batteries that describes all relevant aspects ranging from battery materials, the manufacturing process to the macroscopic cell behavior. These tools are expected to improve understanding and lead to faster, more favorable development processes for novel cell types and to extended lifetime of the batteries. The ITWM team under Dr. Jochen Zausch is focusing on the modeling and simulation of cell performance and aging mechanisms.

The basic components of batteries for e-mobility are complex electrochemical cells. “In our contribution to DEFACTO, we are concentrating on the mechanical aging of the cells, which is caused by volume changes of the battery electrodes,” says Dr. Jochen Zausch, head of the “Electrochemistry and Batteries” team in the “Flow and Materials Simulation” department.

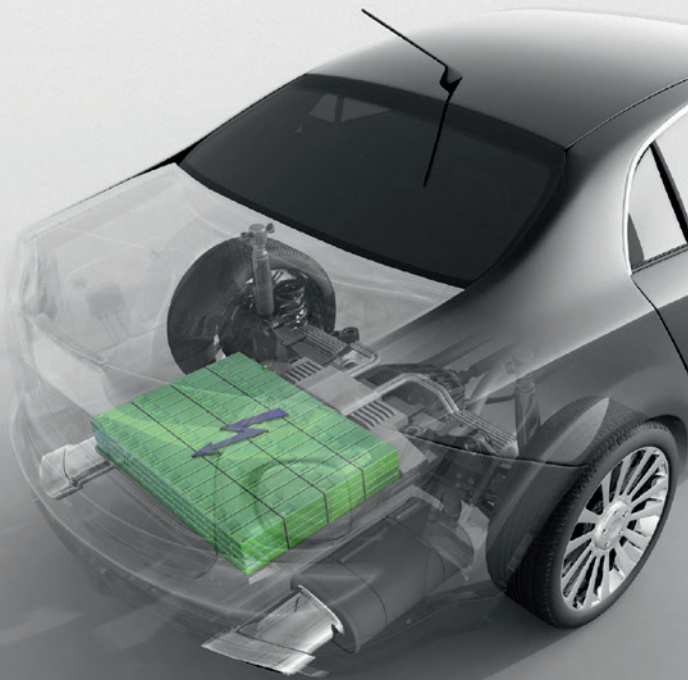
The promising, high-capacity, silicon-containing anodes degrade quickly after only a few charging cycles. The reason for their short cycle-life is the silicon particles in the anode, which expand and contract. This process, which is called “cell breathing,” increases wear due to



*Simulation: Calculated mechanical stresses in a compression experiment of a virtual battery electrode*

cracks and damage. The mechanical stability of the electrodes and thus the charging capacity are gradually reduced. Simplified, these





## “Structure.e”: Faster Charging

Another current e-mobility project that involves the BEST simulation software from ITWM is “Structure.e”. Its goal is to put an end to long waiting times for electric vehicles at charging stations. In this project, which is funded by the German Federal Ministry for Economic Affairs and Energy, Zausch and his team are researching methods that improve the performance and charging capability of lithium-ion batteries. In a large project consortium coordinated by Volkswagen AG, ten companies and research institutions are not only working on the development of new electrode concepts, but also on suitable characterization methods. The work is supported by computer-based simulations, which are developed at ITWM.

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new materials increase the range of the electric vehicle, but at the same time the lifetime of the cells is less than a typical car would require.

### Understanding cell material behavior with ITWM simulations

Zausch and his team get to the root of such problems with the ITWM tool “BEST”, which they use to simulate the electrochemical behavior of the cell. “The big challenge isn’t only about calculating the ideal battery behavior, . We also want to provide for more realism by predicting how the battery properties change over the cell’s lifetime,” says Zausch. This will be achieved by linking and enhancing two ITWM software tools: BEST (for electrochemistry) and FeelMath (for structural mechanics). “Ideally, this microscopic view can then be transferred to the macroscopic scale. We want to

deepen our understanding with regard to material selection, electrode production and processing at the European level.” To promote innovation in e-mobility, the European Commission is funding the DEFACTO project with a total budget of around six million euros. The initiative’s consortium of 13 companies and research institutes from Belgium, France, Germany, Greece and Spain will pursue this ambitious goal through June 2024, with the aim of increasing the competitiveness of European industry.

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