

## ADVANCED COMPUTATIONAL MODELING OF BATTERIES

EDWIN M. KNOBBE<sup>\*</sup>, WOLFGANG A. WALL<sup>†</sup>

<sup>\*</sup> BMW Group, Battery Cell Technology  
80788 München, Germany

[Edwin.Knobbe@bmw.de](mailto:Edwin.Knobbe@bmw.de), <http://www.bmwgroup.com>

<sup>†</sup> Institute for Computational Mechanics, Technical University of Munich  
85747 Garching b. München, Germany  
[wall@lnm.mw.tum.de](mailto:wall@lnm.mw.tum.de), <http://www.lnm.mw.tum.de>

**Keywords:** Multi-Physics, Multi-Scales, Electrochemistry, Batteries.

### ABSTRACT

The objective of this mini-symposium is to bring together people from academia and industry in the area of electrochemical modelling applied to batteries. Special focus of this mini-symposium lies on the integration of computational chemistry within the area of continuum physics. Such an integration provides methods to determine bulk material properties, grain interface phenomena and/or reaction mechanisms. Typical applications of this integration with respect to operating limits are:

- Models to predict the life-time of batteries (automotive and stationary applications).
- Workflow to assess the safety of future batteries with high energy materials (interaction between experiment and simulation).
- Strategies to optimize Fast Charging.

Further topics include - but are not limited to - computational methods and models for:

- Electrochemical modeling and numerical simulation applied to batteries
- Computational methods for electrochemical modeling and performance evaluation
- Integrated approaches for multi-physical problems which couple:
  - thermodynamics,
  - chemistry,
  - electro-magnetism,
  - solid mechanics.
- Computational models for impedance, battery ageing, sub-zero temperature behavior and/or safety evaluation
- System level modeling techniques for batteries (e.g. electromagnetic compatibility, cooling system or battery management systems)
- Parameter estimation & inverse problems for energy storage systems