

Modelling Panel Abstract & Speaker Biography

Microstructurally resolved multiscale models – to study the effects of C/S cathode microstructures used in Li-S batteries

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A better cyclability of Li-S batteries has been achieved only in the recent years by tailoring carbon/sulfur (C/S) cathode with innovative microstructures.¹ However, the impacts of the cathode microstructural properties on the discharge performance still needs to be understood. We report a continuum multi-scale model,² which models the C/S cathodes with detailed microstructural properties such as carbon particle size, pore size, inter-particle porosity between carbon particles and mesoporosity within them. The model is able to provide semi-quantitative predictions about the impacts of C/S microstructures on the discharge performance under different operating conditions. Our continuum model includes some empirical relations to calculate the evolution of some structural properties such as active surface area. Therefore, we have recently developed a novel 3D-Kinetic Monte Carlo (KMC) model based on an in-house Electrochemical Variable Step Size Method (E-VSSM) algorithm,^{3,4} which dynamically resolves the transport, chemical and electrochemical reactions of different polysulfides. The model allows to explore the evolution of the C/S microstructure during discharge in 3D at a mesoscopic scale. The prospects of coupling continuum and KMC models will also be discussed.

References

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3. M. A. Quiroga and A. A. Franco, *J. Electrochem. Soc.*, 162, E73–E83 (2015).
4. G. Blanquer, Y. Yin, M. A. Quiroga, and A. A. Franco, *J. Electrochem. Soc.*, 163, A329–A337 (2016)

Speaker Biography:

Vigneshwaran Thangavel

Education:***2015-Present:***

PhD thesis on 'Multiscale modeling of Lithium sulfur batteries' under the supervision of Prof. Alejandro A. Franco and Dr. Mathieu Morcrette (LRCS, UPJV)

2013-2015:

Erasmus mundus Masters in Material for Energy Storage and Conversion (MESO) (S1: Aix-Marseille University, S2: Warsaw university of Technology, S3 &4: UPJV).

2007-2011:

Bachelor of Technology (B. Tech) in Chemical & Electrochemical Engineering at Central Electrochemical Research Institute (Anna University), Karaikudi, India.

**Summer school:**

4th to 15th July, 2016: College on Multiscale Computational Modeling of Materials for Energy Applications at the Abdus Salam International Center for Theoretical Physics (ICTP), Trieste, Italy.

Work Experience:

2011-2013: R&D Engineer (Design & Process development) at Reem Batteries and Power Appliance Co., Muscat, Oman.

Competencies:

- Modeling of Electrochemical systems;
- Electrochemical characterization techniques (galvanostatic cycling and Electrochemical Impedance spectroscopy);
- BET and Porosimetry analysis;
- UV-Visible spectroscopy.