KEMIJSKI INŠTITUT

Vabilo na Preglov kolokvij / Invitation to the Pregl colloquium

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Velika predavalnica Kemijskega inštituta /
Great Lecture Hall, National Institute of Chemistry;
Hajdrihova 19, Ljubljana

Mesostructure-performance relationships in batteries and fuel cells

Challenging the dogma with multiscale computations and immersive visualization

Optimized design of composite electrodes for batteries and fuel cells is recognized to be of crucial importance, in particular to reach automotive application expectations in terms of performance gain and cost reduction. Such electrodes are currently made of active material or catalysts, additives and binder and the resulting complex porous structure contains an electrolyte. Several conceptual pictures have been developed attempting to capture the influence of these composite electrodes structural properties on the overall cell response: approaches consisting of building up artificial structures capturing the main features of the actual electrodes and approaches based on computer-aided reconstruction of the electrode structure. These two approaches have provided progress on the understanding of batteries and fuel cells operation, but there is still a significant lack of understanding of their structural features (e.g. exact location of the binder) and the impact of the three-dimensional structural anisotropies on the effective transport properties at multiple scales, from the pore and/or particle to the percolated aggregates and/or agglomerates. Defining an appropriate structural picture for the composite electrodes is crucial for a correct interpretation of experimental characterizations but also for optimizing the full cells. In this lecture I discuss a novel computational modelling approach describing the interplays between electrochemical and transport processes at multiple spatial scales. The predictive capabilities of our approach on establishing and optimizing electrode mesostructure-performance relationships are presented within the context of three application examples: (1) discharge and charge mechanisms in Li-O_2 batteries; (2) cyclability of Li-S batteries; (3) membrane degradation and carbon corrosion in PEM Fuel Cells. Finally, the tremendous opportunities opened by the combination of these models with three-dimensional immersive Virtual Reality software for data analysis are discussed on the basis of a recent experience by us on integrating these aspects in our lectures within the Erasmus Master Programme M.E.S.C.

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Vljudno vabljeni / Kindly invited