Sustainability chaired by Bastian Mei/Wim Brilman – room 6

14.15-14.30	*Morphology Evolution during Lithium-based Vertically Aligned Nanocomposite Growth* Daniel Monteiro Cunha (IMS)
14.35-14.50	*High throughput material screening for electrocatalysis* Pauline Roels (VSparticle)
14.55-15.10	*Asymmetric polyelectrolyte multilayer membranes for micropollutant removal* Jurjen Regenspurg (MST)
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Morphology Evolution during Lithium-based Vertically Aligned Nanocomposite Growth, Daniel Monteiro Cunha (IMS)

Ceramics-based nanocomposites is a rapidly evolving research area, as they are currently being used in a wide range of applications. Epitaxial vertically aligned nanocomposites (VANs) offer promising advantages over conventional planar multilayers as key functionalities are tailored by the strong coupling at their vertical interfaces. However, limited knowledge exists of which materials systems are compatible in composite films and which types of structures are optimal for a given functionality. No lithium-based VANs have yet been explored for energy storage, while 3D solid-state batteries offer great promises for enhanced energy and power densities. Although solid-on-solid Kinetic Monte-Carlo simulation (KMCS) models of VAN growth have previously been developed, phase separation was forced into the systems by limiting hopping directions and/or tuning activation energies for hopping. Here, we study the influence of temperature and deposition rate on the morphology evolution of lithium-based VANs, consisting of promising LiMn2O4 cathode and Li0.5La0.5TiO3 electrolyte, by applying a KMCS model with activation energies for hopping obtained experimentally and with minimum restrictions for hopping directions. Although the model considers only the kinetic processes and disregards the thermodynamics of growth that would determine the shape of pillars within the matrix, the trends in pillar size and distribution within the simulated VANs are in good agreement with experiments. This provides an elegant tool to predict the growth of VAN materials, as the experimental activation energies and higher degrees of freedom for hopping result in a more realistic and low computational cost model to obtain accurate simulations of VAN materials.

High throughput material screening for electrocatalysis, Pauline Roels (VSparticle)

Spark ablation technology is a gas phase process for the continuous production of a nano-aerosol of sub-20 nm particles from a very broad range of conductive materials. This physical process only requires electricity, a carrier gas and source material to produce pure, clean nanoparticles without chemical waste. Subsequent forced impaction of the nano-aerosol on a substrate enables local deposition of nanostructured materials. The combination of these two processes results in a novel automated tool for nano-fabrication.

An essential step in hydrogen production by electrochemical water splitting is the energy demanding oxygen evolution (OER). Here, it will be shown how material libraries for oxygen evolution electrocatalysis can be created by nano-aerosol deposition on a high-throughput chip (an array of 8x8 dots was printed onto a nickel substrate). The importance of electrocatalyst morphology will be revealed and particularly the effect of the deposition time and composition on the OER was tested. Using the screening approach a fast optimization of the cell potential was obtained using nanoparticle Ni/Fe ratio and deposition time as variables.

Generally, it is expected that spark ablation might significantly reduce catalyst development time.

Asymmetric polyelectrolyte multilayer membranes for micropollutant removal, Jurjen Regenspurg (MST)

New membrane materials are urgently needed to address the increasing concentrations of harmful organic micropollutants (e.g. pharmaceuticals, pesticides and plasticizers) in our surface and drinking water. Conventional wastewater treatment plants (WWTPs) are not capable of fully removing micropollutants from wastewater. Using the densest available membranes micropollutants can be removed but this comes with many disadvantages, making it too costly to apply in WWTPs. Asymmetric polyelectrolyte multilayer membranes tackle these disadvantages. First, a highly permeable polyelectrolyte multilayer is coated on a support membrane to close the pores. Secondly, a dense separation layer of only 4 nm in thickness is coated for selectivity. This way of coating results in asymmetric polyelectrolyte multilayer membranes that retain 98% of micropollutants while maintaining high permeabilities. By overcoming the disadvantages of current membrane techniques asymmetric polyelectrolyte membranes have a great potential for the use in clean and safe drinking water production.

Islanded power-to-ammonia-to-power for electricity storage, Kevin Rouwenhorst (CPM)

Energy storage in hydrogen is often proposed in a future scenario with intermittent power sources, such as solar and wind. However, hydrogen storage is difficult and chemical hydrogen carriers are required for long-term storage, such as ammonia. This carbon-free hydrogen carrier is primarily used as a fertilizer, increasing the population from 1 billion people in 1900 to 7 billion people in 2000. Nowadays, ammonia is also considered as an energy storage vector, to store electrolysis-based hydrogen. In this study, the state-of-the-art of small-scale power-to-ammonia-to-power systems (1-10 MW) is reviewed and an process is designed. In such an islanded power system, all electricity is produced from renewables (solar and wind) and storage in batteries (short-term) & chemicals (long-term) is introduced to account for intermittency of renewables, as well as fluctuations in demand. In a generic location in the Netherlands, it is possible to operate such an islanded energy system at a cost of about 0.30-0.35 € kWh^{-1}.