Modelling and optimizing electrolyzers across scales

The climate is changing and as a reaction to this we must push for a sustainable society as fast as possible. Fluctuating renewable energy and energy conversion is central to this transition. Energy conversion can balance the fluctuations and at the same time produce fuels and chemicals, i.e. power to X, for sectors in which direct electrification is not possible. In these power to X plants, a hydrogen producing electrolyzer will thus also be the major energy converter, as hydrogen is the energy carrier in all X's. It is thus the electrolyzers, which must be able to dynamically adjust the production of hydrogen. As these plants have barely been build and their dynamic behaviour barely understood, it is clear that a vast amount of engineering lies ahead, and it is clear that if any predictions on the behaviour of these plants can be made, it would be of great benefits for the engineers, who are to design and optimize the materials, cells, stacks and systems. Because to optimize the electrolyzers, they must be understood at various levels, as each design choice influence the behaviour across levels, and optimizing one part will influence others.

This lecture will cover our research on developing multiscale modelling concept to span from materials scale to energy system scale. To understand the implication of choices on various levels, we need to combine materials scale, microstructural scale with cell, stack and system scale in a joint framework. The objective is to systematically assemble theoretical and empirical models to build tools for designing and optimizing the future power to X plants, but also to guide the technological advancements needed. Scientifically, the challenge is to formulate the mathematical multiscale concepts, which allows this type of computations. The lecture will cover the researched concepts and perspectives on future research.