

Modelling approaches to guide the design of photo-electrochemical water splitting devices

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The functionality of photo-driven electrochemical devices relies on complicated and coupled multi-physics processes, happening on multiple temporal and spatial scales. Device modelling can efficiently and actively support the choice of the most interesting – in terms of efficiency, cost, robustness, scalability, and practicability – conceptual design pathways, material choices, and operating approaches.

Models of photo-driven electrochemical devices and components can incorporate a wide range of physical phenomena and complexity. I will discuss the merit of and lessons learned from device models incorporating different degree of complexity and dimensionality. This will include i) steady and transient 0-dimensional model for the discussion of material choices, degradation and device integration, ii) steady 1-dimensional models to understand the semiconductor-electrolyte interface's role on the performance of photocatalytic and photoelectrochemical device designs, iii) steady 2-dimensional models for the discussion of the effect of temperature and the management on the performance, and iv) 3-dimensional model for the detailed understanding of transport limitations in morphologically-complex photoelectrodes.

Renewable energy driven non-thermal chemistry for the production of fuels and chemicals

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Renewable energy generation by means of wind or from solar radiation through photovoltaics or concentrated solar power will continue to increase its share in the energy mix. Intermittency (due to e.g. day/night cycle), the regional variation of these energy sources, and penetration of renewable energy into other sectors than electricity (e.g. the chemical industry) requires means to store, transport and convert energy on a large scale.

A promising option is the synthesis of chemicals and synthetic fuels (easily deployable within the present fossil fuels infrastructure) from raw feedstock using renewable energy. A truly circular economy requires that the raw materials are the thermodynamically most stable molecules such as water (H₂O), carbondioxide (CO₂) and nitrogen (N₂) to generate, e.g. hydrogen, hydrocarbons and ammonia. In this talk it will be highlighted how non-thermal chemistry can potentially combine compatibility with e.g. intermittency and localized production to activate these molecules with ultimate energy efficiency, essentially due to the use of preferential vibrational excitation, electric fields or non-thermal excitation, etc. This will cause inherently out-of-equilibrium processing conditions that can achieve selectivity and higher throughputs in the reaction processes.