

Computational Engineering of Solid Oxide Cell Materials

Abstract for inaugural lecture

Professor Ming Chen

Solid oxide cells (SOCs) are electrochemical devices, converting chemical energy of fuels into electricity and heat, or vice versa. The SOC technology has a great potential to become a key technology in enabling the transition towards renewables. The production of SOC cells or stacks involves several sintering steps with a maximum temperature of 1300 – 1400 °C, whereas the operation takes place in a range of 600 – 900 °C. High temperature accelerates the sintering process and the kinetics of the various electrochemical reactions, but also promotes atomic diffusion and microstructure evolution, and in some cases detrimental reactions, limiting the performance and lifetime and to some extent the wide spread application of the technology.

Professor Ming Chen will give a lecture discussing the computational efforts devoted to developing better SOC materials & microstructures. He will first touch upon the principles of SOCs, and afterwards focus on different aspects of computational modeling of SOC materials, from classical computational thermodynamics & phase diagrams for material composition optimization, to modelling diffusion induced phase transformation & interface reactions for process optimization, and eventually to modelling 3D microstructure evolution for microstructure engineering. These will be combined with actual examples illustrating how the modelling has helped developing high performing and durable SOCs.