Area D: Characterization and Modelling

Symposium D8:

Title: **Multiscale and Multiphysics Modelling of Materials, Processes and Products**		
Organizer	***Institution***	***Contact email***
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Abstract

This symposium is dedicated to multiscale and multiphysics modelling of processing-microstructure-property relation of materials, its uncertainty quantification and its improvement of predictability.

Multiscale and multiphysics modelling of materials, processes and products provide comprehensive fundamental understanding of the underlying mechanisms and allow for numerical prototyping of materials and material-driven innovations in science and industry. Modelling and simulation techniques are well established at each individual scale (quantum, atomistic, mesoscale and continuum) and significant progress in development of appropriate coupling and linking has been achieved. Nevertheless, there still remain significant challenges that limit the quantitative and predictive capability of multiscale modelling and simulation tools. Beside focusing on these challenges, the symposium is also devoted to modelling the evolution of the atomistic-, nano- and microstructure during processing – typically driven by multiphysical phenomena – and its effect on the structural and functional material properties. The symposium also covers hybrid modelling in the sense of a combination of physical-based and artificial intelligence-driven models covering multiscale or multiphysics problems.

We particularly invite discussions, reports of implementation and application of multiscale or multi-physics modelling including at least two scale levels or physical phenomena. The symposium is not restricted to any kind of material (structural materials, functional materials, energy materials, composites, soft matter, …) or field of application (mechanical engineering, automotive/aviation, microelectronics, energy, chemistry, metallurgy, …).

The topics to be covered by the symposium are:

- Approaches bridging different spatial or temporal scales
- Concurrent, hierarchical and hybrid multiscale schemes
- Modelling complex multiscale hierarchies
- Modelling microstructure-property relations
- Multidisciplinary and multi-science problems
- Approaches involving different physics (e.g. magnetic, electric, electronic, thermal, mechanical, thermodynamic, kinetic)
- Combining physical-based and artificial intelligence-driven models
- IC-MPPE (Integrated Computational Materials, Process, and Product Engineering)
- Coarse grained methods
- Ab-initio methods
- Molecular dynamics
- Atomistic-based continuum methods
- Thermodynamic- and kinetic-based methods
- Multi-scale validation
- Uncertainty prediction