Area B: Structural Materials
Symposium B9:

Title : **Theory-guided Development Structural Materials**		
Organizer	***Institution***	***Contact email***
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Abstract

Scope: The goal of this symposium is to present state-of-the-art and thereby to identify and to propose new directions of theory-guided research to design future structural materials.

Description: In recent years, computer-aided materials design has become an integral of the field of structural materials. It includes theoretical tools that provide an unprecedented insights into materials well beyond experimental resolution. But research in modern materials science often requires a close integration of computation and experiments in order to fundamentally understand and design the materials properties of new structural materials. In particular, a controlled experimental testing of theoretical hypothesis allows for explaining complex multi-scale structure-composition-property relationships and, eventually, a systematic discovery of novel materials.

In this symposium we aim on bringing together materials modelers working on various scales, from electronic structure over atomistic description, up to mesoscale dislocation dynamics, phase field and CALPHAD methods. In recent years, the availability of large datasets combined with the improvement in algorithms and the exponential growth in computing power led to an unprecedented surge of interest in the topic of machine learning. This rapidly developing scientific field offers also unique opportunities to address grand challenge problems in materials science. We welcome contributions which provide explanations for long standing problems in design of structural materials as well as those exploring new horizons and proposing novel material systems and concepts. Particularly sought are contributions bridging theory and experiment, nevertheless purely theoretical contributions are equally welcome.

This symposium will cover, but is not limited to, the following range of topics:

- Ab initio simulations
- Atomistic modeling
- Data-driven approaches in atomistic simulations, including ML/AI

- Coarse-graining techniques
- Dislocation-based modeling
- Multi-scale modeling
- Experimental techniques for validation of multi-scale models