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Computational Design of Complex Structural Alloys

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Deadline for manuscript submissions:
closed (20 March 2019)

Message from the Guest Editors

Modelling tools have recently developed into a such stage where they are of a valuable help to steer the development and optimisation of novel structurally complex alloys. Still, in order to obtain picture which is of practical relevance at experimental length-scales, information from several levels of modelling insight must be combined. Quantum mechanical calculation provide description of the inter-atomic interactions on the very fundamental level; atomistic methods are suitable for studying extended defects (e.g., grain boundaries, dislocations, cracks etc.) and their mutual interactions; finally, mesoscopic continuum thermodynamics methods are suitable for describing the microstructural evolution.

The intention of this special issue is to attract contributions combining ab initio, atomistic (molecular statics/dynamics or Monte Carlo) and thermodynamic (phase field and CALPHAD) modelling approaches with experimental works. The contribution should show the state-of-the-art in predicting composition and microstructure and thus to not only provide explanation for various phenomena occurring in multi-phase structural alloys, but also to guide their further improvement.

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Message from the Editor-in-Chief

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