EUROMAT 2017/ Symposia Structure/Area D

D.8

Title: Ab initio models for thermodynamic and elastic properties of advanced materials

Organizer	Institution	Contact email
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Summary

Quantum-mechanical density functional *ab initio* computational methods have now achieved an unprecedented level of accuracy and reliability in predicting properties of a broad variety of materials. *Ab initio* calculations provide deep insight in the fundamentals of electronic structure of a material and its excited electronic states, as well as atomistic and magnetic dynamics, controlling the phase stability and properties at elevated temperatures, up to the melting point. Owing to their universality and reliability, quantum-mechanical approaches have become the method of choice not only for studying existing materials but also for designing new materials. In particular, whenever experimental data are missing, density functional and other quantum-mechanical calculations deliver information required for constructing higher-level mathematical models and algorithms, including semi-empirical thermodynamic calculations of phase diagrams (CALPHAD), atomistic and continuum methods, and multi-scale models for simulating complex microstructural features like defects and dislocations. The scope of the symposium includes *ab initio* and other quantum-mechanical models, and applications of these models to the treatment of thermodynamic and mechanical, for example elastic, properties of materials. Contributions are invited that cover both the methodological developments as well as a variety of applications to a range of materials including:

(i) Nickel and cobalt based superalloys
(ii) High entropy alloys (HEAs)
(iii) Advanced steels
(iv) Light-weight structural materials
(v) Advanced functional materials
(vi) Dislocations and defects in metals and alloys, including HEAs
(vii) Magnetic metals and alloys
(viii) Atomistic and magnetic dynamics and thermodynamics of advanced materials
(ix) Ab initio based predictive multiscale models

Invited speakers at the symposium are:

Prof. **Igor A. Abrikosov** (Linköping University, Sweden)
Prof. **Ralf Drautz** (Ruhr-Universität Bochum, Germany)
Dr. **Mihai-Cosmin Marinica** (CEA Saclay, France)
Prof. **Jörg Neugebauer** (Max-Planck Institute for Iron Research, Germany)