

EUROMAT 2021

EUROPEAN CONGRESS AND EXHIBITION
ON ADVANCED MATERIALS AND PROCESSES

WWW.EUROMAT2021.FEMS.EU

12. - 16. SEPTEMBER 2021

GRAZ, AUSTRIA

ASMET
THE AUSTRIAN SOCIETY FOR
METALLURGY AND MATERIALS

FEMS 30
FEDERATION OF EUROPEAN
MATERIALS SOCIETIES
1987 - 2017
www.FEMS.org

Area D: Characterization and Modelling

Symposium D7:

Title: Integrated Computational Materials Engineering – Interoperability, Simulation Platforms and Applications

Organizer	Institution	Contact email
Georg J. Schmitz	ACCESS e.V. Aachen, Germany	G.J.Schmitz@micress.de
Javier Llorca	IMDEA Materials, Madrid, Spain	javier.llorca@imdea.org
Nicola Mazari	EPFL Lausanne, Switzerland	nicola.marzari@epfl.ch
Christian Haase	RWTH Aachen University, Germany	Christian.Haase@iehk.rwth-aachen.de

Abstract

Integrated Computational Materials Engineering, ICME and its use in materials and process design drastically decreases development times of new products. By its name and by its nature ICME draws on the combination – coupling and linking - of a diverse variety of models and tools. Monolithic tools are unlikely to be capable of tackling the host of phenomena occurring during processing and service life-cycle of materials. Accordingly, there is a need for modular and freely configurable workflows orchestrating the simultaneous or consecutive execution of a variety of tools. Contributions thus are sought addressing following topics:

- Interoperability, standardization, and ontologies
- Materials simulation platforms and workflows
- Integration of experimental characterization into simulation workflows

We further invite discussions, implementation reports and illustrations of applications of materials modelling workflows - directly or indirectly - integrating multiple (at least two) different simulation tools and/or model worlds selected from

- Discrete models and their practical applications (electronic & atomistic modelling, molecular dynamics, dislocation-dynamics...)
- Continuum materials models and their applications (phase-field, phase-field crystal, crystal-plasticity, thermodynamics & kinetics...)
- Phenomenological models (e.g. microstructure property relations)
- Artificial Intelligence (AI) models in materials science and engineering

The symposium does not restrict to specific materials and especially seeks for contributions related to applications (mobility, health, communication, energy, public infrastructure...).