

# Open Simulation Platforms in the European Multi-Scale Modelling Cluster

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## ABSTRACT

ICME is poised to change the way materials are developed based on concurrent design of process, structure, property and performance. The success of ICME hinges on the availability of capable computational modelling tools that can be readily integrated in complex workflows. This requires advancing the multiscale science of coupling (concurrent) and linking (hierarchical sequential) multiscale modelling paradigms. At the same time, this also requires establishing interoperability between different computational tools acting on various scales and models to facilitate their integration in ICME workflows. The scope of this presentation is to give an overview of recent developments in Europe that cover interoperability and materials modelling meta-data stemming from recent European actions. The aim is to advance so-called Open Simulation Platforms (OSP) that provides an open standard for interoperability and integration. The developments have been carried out under the umbrella of the European Materials Modelling Council EMMC and the European MultiScale Modelling Cluster (EU-MSM). The EU-MSM brings together 6 different EU supported projects that have the overarching goal to collaborate on developing data standards and interoperability interfaces for various simulation tools and creating integrated multiscale modelling environments for nano-enabled materials. These activities aim to reach a consensus on the best approaches to boost ICME and the industrial application of Multiscale Materials Modelling in Europe.

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## REFERENCES

- [1] European Materials Modelling Council (EMMC): [www.emmc.info](http://www.emmc.info)
- [2] EU project MoDeNa: Modelling of morphology Development of micro- and Nanostructures <http://modena.units.it/>
- [3] EU project Deepen: From atom-to-Device Explicit simulation Environment for Photonics and Electronics Nanostructures <http://www.nmp-deepen.eu/>
- [4] EU project Symphony: Simulation framework for multi-scale phenomena in micro- and nanosystems <http://www.simphony-project.eu>
- [5] EU project MMP: Multiscale Modelling Platform: Smart design of nano-enabled products in green technologies <http://www.mmp-project.eu/>
- [6] EU Project NanoSim: A Multi-scale Simulation-Based Design Platform for Cost-Effective CO2 Capture Processes using Nano-Structured Materials <http://www.sintef.no/Projectweb/NanoSim>
- [7] EU- Coordination and Support Action ICMEg: [www.icmeg.eu](http://www.icmeg.eu) (Accessed Aug. 2015) see also G.J.Schmitz and U.Prahl: Integrating Materials Manufacturing Innovation 2014, 3:2S.