## Simulation Methods on Virtual Laboratories for Characterization of Functionalized Nanostructures

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## Abstract

Within the emerging integrative concept of IoT (Internet of Things) and IIoT (Industrial Internet of Things) that are paving the way towards Digital Manufacturing Technologies and the next paradigm shift of Industry 4.0, R&D Laboratories have to be at the forefront of the transformation.

Using remotely the existing top R&D Laboratories facilities would become soon common practice, but for now basic training, teaching and R&D collaboration on specific issues can be successfully deployed. Thus, the necessary multi-disciplinary and trans-disciplinary expertise for running on the Digital Manufacturing Era to come will be properly achieved.

A first step on producing functionalized materials to be integrated on smart applications is to properly settle their multi-physic models as to adequately consider their properties during designing the processing, post-processing and controlling phases based on successive simulations.

Serving this purpose COMSOL Multiphysics® is a core-function software used for a proper and deeper understanding of the complex-dynamic relationship existing among physics, processing and control on designing and simulating specific applications.

During the description, characterization and process simulation phases for different R&D Laboratory equipment and installations the main modules of COMSOL Multiphysics® were extensively used, as well as its add-ons (LiveLink<sup>™</sup> for SolidWorks®, LiveLink<sup>™</sup> for CATIA, LiveLink<sup>™</sup> for Excel, LiveLink<sup>™</sup> for MATLAB®)

The core physic processes related to the lab installation (e.g., Mass Spectrometer) were described adapting the existing COMSOL Multiphysics® models to the actually installed lab equipment data

All experimental data related to the process (characterization) are archived in dedicated modules for each specific installation. These will be further adapted to the different experimental arrays.

## Figures used in the abstract

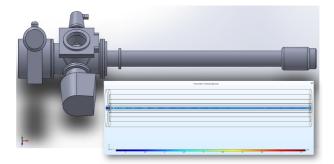


Figure 1: Ion Gun assembly within Mass Spectrometry installation.